



06-26-00

526 Rec'd PCT/PTO 23 JUN 2000

PCT

U.S. DEPARTMENT OF COMMERCE PATENT AND TRADEMARK OFFICE (REV 11-98)		ATTORNEY'S DOCKET NUMBER P02005US0
TRANSMITTAL LETTER TO THE UNITED STATES DESIGNATED/ELECTED OFFICE (DO/EO/US) CONCERNING A FILING UNDER 35 U.S.C. 371		U.S. APPLICATION NO. (if known, see 37 CFR 1.5) 09/582486
INTERNATIONAL APPLICATION NO. PCT/GB98/03860	INTERNATIONAL FILING DATES 24 December 1998	PRIORITY DATE CLAIMED 24 December 1997 24 June 1998
TITLE OF INVENTION MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE		
APPLICANT(S) FOR DO/EO/US Christopher Joseph Schofield; Jack Edward Baldwin; Peter L. Roach; Matthew D. Lloyd; Karl Harlos; Inger Andersson; Janos Hajdu; Anke S. Terwisscha Van Scheltinga; Karin Valegard; and S. Ramaswamy		
Applicant herewith submits to the United States Designated/Elected Office (DO/EO/US) the following items and other information:		
<ol style="list-style-type: none">1. <input checked="" type="checkbox"/> This is a FIRST submission of items concerning a filing under 35 U.S.C. 3712. <input type="checkbox"/> This is a SECOND or SUBSEQUENT submission of items concerning a filing under 35 U.S.C. 371.3. <input type="checkbox"/> This express request to begin national examination procedures (35 U.S.C. 371 (f)) at any time rather than delay examination until the expiration of the applicable time limit set in 35 U.S.C. 371 (b) and PCT Articles 22 and 39(1).4. <input checked="" type="checkbox"/> A proper Demand for International Preliminary Examination was made by the 19th month from the earliest claimed.5. <input checked="" type="checkbox"/> A copy of the International Application as filed (35 U.S.C. 371 (c)(2))<ol style="list-style-type: none">a. <input checked="" type="checkbox"/> is transmitted herewith (required only if not transmitted by the International Bureau).b. <input type="checkbox"/> has been transmitted by the International Bureau.c. <input type="checkbox"/> is not required, as the application was filed in the United States Receiving Office (RO/US).6. <input type="checkbox"/> A translation of the International Application into English (35 U.S.C. 371 (c)(2)).7. <input checked="" type="checkbox"/> Amendments to the claims of the International Application under PCT Article 19 (35 U.S.C. 371 (c)(3))<ol style="list-style-type: none">a. <input type="checkbox"/> are transmitted herewith (required only if not transmitted by the International Bureau).b. <input type="checkbox"/> have been transmitted by the International Bureau.c. <input type="checkbox"/> have not been made; however, the time limit for making such amendments has NOT expired.d. <input checked="" type="checkbox"/> have not been made and will not be made.8. <input type="checkbox"/> A translation of the amendments to the claims under PCT Article 19 (35 U.S.C. 371 (c)(3)).9. <input type="checkbox"/> An oath or declaration of the inventor(s) (35 U.S.C. 371 (c)(4)).10. <input type="checkbox"/> A translation of the annexes to the International Preliminary Examination Report under PCT Article 36 (35 U.S.C. 371 (c)(5)).		
Items 11. to 16. below concern document(s) or information included:		
<ol style="list-style-type: none">11. <input checked="" type="checkbox"/> An Information Disclosure Statement under 37 CFR 1.97 and 1.98.12. <input type="checkbox"/> An assignment document for recording. A separate cover sheet in compliance with 37 CFR 3.28 & 3.31 is included.13. <input checked="" type="checkbox"/> A FIRST preliminary amendment. <input type="checkbox"/> A SECOND or SUBSEQUENT preliminary amendment.14. <input type="checkbox"/> A substitute specification.15. <input checked="" type="checkbox"/> A change of power of attorney and/or address letter.16. <input checked="" type="checkbox"/> Other items or information: Sequence Listing and Diskette		

EXPRESS MAIL LABEL NO. EK102712205US

U.S. APPLICATION NO. (if known, see 37 CFR 1.5)		INTERNATIONAL APPLICATION NO.		ATTORNEY'S DOCKET NUMBER	
09/582486		PCT/GB98/03860		P02005US0	
17. <input checked="" type="checkbox"/> The following fees are submitted:				CALCULATIONS PTO USE ONLY	
BASIC NATIONAL FEE (37 CFR 1.492 (a) (1) – (5)): <input type="checkbox"/> Neither international preliminary examination fee (37 CFR 1.482) nor international search fee (37 CFR 1.445(a)(2)) paid to USPTO and International Search Report not prepared by the EPO or JPO <input checked="" type="checkbox"/> International preliminary examination fee (37 CFR 1.482) not paid to USPTO but International Search Report prepared by the EPO or JPO <input type="checkbox"/> International preliminary examination fee (37 CFR 1.482) not paid to USPTO but international search fee (37 CFR 1.445(a)(2)) paid to USPTO <input type="checkbox"/> International preliminary examination fee paid to USPTO (37 CFR 1.482) but all claims did not satisfy provisions of PCT Article 33(1)-(4) <input type="checkbox"/> International preliminary examination fee paid to USPTO (37 CFR 1.482) and all claims satisfied provisions of PCT Article 33(1)-(4)					
ENTER APPROPRIATE BASIC FEE AMOUNT =				\$970.00	
Surcharge of _____ for furnishing the oath or declaration later than <input type="checkbox"/> 20 <input type="checkbox"/> 30 months from the earliest claimed priority date (37 CFR 1.492 (e)).					
CLAIMS	NUMBER FILED	NUMBER EXTRA	RATE		
Total claims	232 - 20 =	212	X 18	3,816.00	
Independent claims	13 - 3 =	10	x 78	780.00	
MULTIPLE DEPENDENT CLAIM(s) (if applicable)			x	-0-	
TOTAL OF ABOVE CALCULATIONS =				5,566.00	
Reduction of ½ for filing by small entity, if applicable. Verified Small Entity Statement must also be filed (Note 37 CFR 1.9, 1.27, 1.28).					
SUBTOTAL =				5,566.00	
Processing fee of _____ for furnishing the English translation later than <input type="checkbox"/> 20 <input type="checkbox"/> 30 months from the earliest claimed priority date (37 CFR 1.492 (f)).				+	
TOTAL NATIONAL FEE =				5,566.00	
Fee for recording the enclosed assignment (37 CFR 1.21 (h)). Assignment must be accompanied by appropriate cover sheet (37 CFR 3.28, 3.31) (_____ per property).				+	
TOTAL FEES ENCLOSED =				\$5,566.00	
				Amount to be:	
				Refunded	
				Charged	
a. <input type="checkbox"/> A check in the amount of _____ to cover the above fees is enclosed. b. <input checked="" type="checkbox"/> Please charge my Deposit Account No. <u>06-2375</u> in the amount of <u>\$5,566.00</u> to cover the above fees. A duplicate copy of this sheet is enclosed. c. <input checked="" type="checkbox"/> The Commissioner is hereby authorized to charge any additional fees which may be required or credit any overpayment to my Deposit Account No. <u>06-2375</u> . A duplicate copy of this sheet is enclosed.					
NOTE: Where an appropriate time limit under 37 CFR 1.494 has not been met, a petition to revive (37 CFR 1.137 (a) or (b)) must be filed and granted to restore the application to pending status.					
SEND ALL CORRESPONDENCE TO:					
Melissa D. Schwaller Fulbright & Jaworski L.L.P. 1301 McKinney, Suite 5100 Houston, TX 77010-3095					
<i>Melissa D. Schwaller</i> Melissa D. Schwaller 46,089 _____ REGISTRATION NUMBER					
6-23-00					

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Serial No.:	To be assigned	§ Docket No.: P02005US0
Filing Date:	June 16, 2000	§
Applicants:	C. Schofield <i>et al.</i>	§
Title:	Modified Deacetoxycephalosporin C Synthase (DAOCS) and X-Ray Structure	§
		§
		§
		§
		§
		§

Assistant Commissioner for Patents
Washington, D.C. 20231

Dear Sir:

Applicants respectfully request the entry of the present statement in regard to the enclosed sequence listing in the above-referenced application. The submitted materials include a computer readable form and paper copy of a sequence listing for the sequence found in the application (SEQ ID NO: 1). Applicants state the information recorded in the computer readable form of the sequence listing is identical to the written sequence listing. Applicants also state that the submission, filed in accordance with 37 CFR 1.821(g), does not include new matter. The sequence found in the sequence listing is identical to that found in the application.

If you have any questions regarding the above-referenced application, please do not hesitate to contact me.

Respectfully submitted,

Melissa D. Schwaller

Melissa D. Schwaller, Ph.D.
Registration No. 46,089

Date: 6-23-00

Fulbright & Jaworski L.L.P.
1301 McKinney, Suite 5100
Houston, Texas 77010-3095
(713) 651-7732

SEQUENCE LISTING

<110> SCHOFIELD, Christopher J.
 BALDWIN, Jack E.
 LLOYD, Matthew D.
 HARLOS, Karl
 ANDERSSON, Inger
 TERWISSCHA VAN SCHELTINGA, Anke S.
 VALEGARD, Karin
 RAMASWAMY, S.

<120> MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND
 X-RAY STRUCTURE

<130> 08004624

<140> PCT/GB98/03860
 <141> 1998-12-24

<150> 9727370.0
 <151> 1997-12-24

<150> 9813644.3
 <151> 1998-06-24

<160> 1

<170> PatentIn Ver. 2.1

<210> 1
 <211> 311
 <212> PRT
 <213> Streptomyces clavuligerus

<400> 1
 Met Asp Thr Thr Val Pro Thr Phe Ser Leu Ala Glu Leu Gln Gln Gly
 1 5 10 15
 Leu His Gln Asp Glu Phe Arg Arg Cys Leu Arg Asp Lys Gly Leu Phe
 20 25 30
 Tyr Leu Thr Asp Cys Gly Leu Thr Asp Thr Glu Leu Lys Ser Ala Lys
 35 40 45
 Asp Leu Val Ile Asp Phe Phe Glu His Gly Ser Glu Ala Glu Lys Arg
 50 55 60
 Ala Val Thr Ser Pro Val Pro Thr Met Arg Arg Gly Phe Thr Gly Leu

65		70		75		80
Glu Ser Glu Ser Thr Ala Gln Ile Thr Asn Thr Gly Ser Tyr Ser Asp						
	85		90		95	
Tyr Ser Met Cys Tyr Ser Met Gly Thr Ala Asp Asn Leu Phe Pro Ser						
	100		105		110	
Gly Asp Phe Gly Arg Ile Trp Thr Gln Tyr Phe Asp Arg Gln Tyr Thr						
	115		120		125	
Ala Ser Arg Ala Val Ala Arg Glu Val Leu Arg Ala Thr Gly Thr Glu						
	130		135		140	
Pro Asp Gly Gly Val Glu Ala Phe Leu Asp Cys Glu Pro Leu Leu Arg						
	145		150		155	160
Phe Arg Tyr Phe Pro Gln Val Pro Glu His Arg Ser Ala Glu Glu Gln						
	165		170		175	
Pro Leu Arg Met Ala Pro His Tyr Asp Leu Ser Met Val Thr Leu Ile						
	180		185		190	
Gln Gln Thr Pro Cys Ala Asn Gly Phe Val Ser Leu Gln Ala Glu Val						
	195		200		205	
Gly Gly Ala Phe Thr Asp Leu Pro Tyr Arg Pro Asp Ala Val Leu Val						
	210		215		220	
Phe Cys Gly Ala Ile Ala Thr Leu Val Thr Gly Gly Gln Val Lys Ala						
	225		230		235	240
Pro Arg His His Val Ala Ala Pro Arg Arg Asp Gln Ile Ala Gly Ser						
	245		250		255	
Ser Arg Thr Ser Ser Val Phe Phe Leu Arg Pro Asn Ala Asp Phe Thr						
	260		265		270	
Phe Ser Val Pro Leu Ala Arg Glu Cys Gly Phe Asp Val Ser Leu Asp						
	275		280		285	
Gly Glu Thr Ala Thr Phe Gln Asp Trp Ile Gly Gly Asn Tyr Val Asn						
	290		295		300	
Ile Arg Arg Thr Ser Lys Ala						
	305		310			

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

APPLICANT: C. J. SCHOFIELD ET AL. : DOCKET NO.
: P02005US0

FILING DATE: TO BE ASSIGNED :
:

SERIAL NO.: TO BE ASSIGNED : Gr : To be
: assigned

TITLE: MODIFIED DEACETOXYCEPHALOSPORIN :
C SYNTHASE (DAOCS) AND X-RAY : Examiner:
STRUCTURE : To be assigned

Assistant Commissioner of Patents

Washington, D.C. 20231

FIRST PRELIMINARY AMENDMENT

Dear Sir:

Please enter the following amendments to the claims prior to the examination of the application.

IN THE CLAIMS:

Please amend the claims as follows:

1. (amended) Deacetoxycephaloporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B [herein].

2. (amended) DAOCS in the form of a complex with a metal, [e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor,] having a structure designated by the X-ray co-ordinates [herein] of structure B.

3. (amended) DAOCS as claimed in claim [2] 28, wherein the substrate is selected from the group consisting of penicillin N, penicillin G, 2-oxoglutarate or dioxygen [,and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide].

4. (amended) [Use of the three-dimensional structure of DAOCS for the modification of] A method of modifying DAOCS or other related 2-oxoglutarate dependent [enzyme] enzymes comprising referring to the three-dimensional structure of DAOCS to select the modification of said enzymes.

5. (amended) [Use as claimed in] The method of claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the 7 α -methoxy group into cephamycin C.

6. (amended) [Use as claimed in] The method of claim 5, [for] wherein the modification of DAOCS, DACS or DAOC/DACS is such that they accept unnatural substrates more efficiently than the wild type enzymes.

7. (amended) [Use as claimed in] The method of claim 5, [for] wherein the modification of DAOCS, DACS, DAOC/DACS is such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

8. (amended) [Use as claimed in] The method of claim 6, wherein the unnatural substrates are penicillins [including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain].

9. (amended) [Use as claimed in] The method of claim 6, wherein the unnatural substrate is a cephalosporin.

10. (amended) [Use as claimed in] The method of claim 6, wherein the unnatural substrate is an amino acid or a peptide.

11. (amended) [Use as claimed in any one of claims] The method of claim 6[-8], wherein [penicillin G, penicillin V, another] unnatural substrate [or penicillin N] is converted to a cephalosporin [or exomethylene cephalosporin].

12. (amended) An enzyme having significant [(as herein defined)] sequence similarity to DAOCS, wherein the side chain binding site of [penicillin N or] DAOC is modified and at least one amino acid residue [and] at [at least] one or more of the following sites [at least one amino acid residue] selected from the group consisting of Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, and Asn304; is changed to another amino acid residue or is deleted[: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303,

and Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above].

13. (amended) An enzyme having significant [(as herein defined)] sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of [penicillin N or] DAOC is modified [and at] at [least] one or more of the following amino acid residues selected from the group consisting of Ile 88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg 306, and Arg307; is changed or deleted: [Ile 88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg 306, and Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above].

14. (amended) An enzyme according to claim 12 [or claim 13] which is a [mutant] modification of DAOCS or DACS or DAOC/DACS.

15. (amended) An enzyme [as claimed in any one of claims 12-14] having significant sequence similarity to DAOCS, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues [specified in claims 12 and 13] selected from the group consisting of Thr72, Arg74, Arg75, Ile88, Glu156, Leu158, Arg160, Arg162, Phe164, Met180, Leu186, Ser187, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; Ile305, Arg 306, and Arg307 is changed or deleted [and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above].

16. (amended) An enzyme as claimed in [any one of claims] claim 12[-15], wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

17. (amended) A [gene] polynucleotide encoding [for] the enzyme of [any one of claims] claim 12[-16].

18. (amended) A micro-organism capable of expressing the [gene] polynucleotide of claim 17 under fermentation conditions.

19. (amended) [Use of] The method of using the micro-organisms of claim 18 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

20. (amended) [Use as claimed in] The method of claim 19, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway [including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase].

22. (amended) A method as claimed in claim 21 wherein the said other related 2-oxoglutarate dependent enzyme or related enzyme is 1-aminocyclopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3 β -hydroxylase, hyoscyamine 6 β -hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ -butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavamate synthase, and oxygenase enzyme involved in the biosynthesis of carbapenems, the [so called] ethylene forming enzyme from *Pseudomonas syringe*, p-

hydroxyphenylpyruvate dioxygenase, [and] or an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

23. (amended) A method as claimed in claim 21 [or 22] wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites [defined in claim 12 or 13] selected from the group consisting of Thr72, Arg74, Arg75, Ile 88, Glu156, Leu158, Arg160, Arg162, Phe164, Met180, Leu186, Ser187, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; Ile305, Arg 306, and Arg307; or using the following information for the design [or] of an inhibitor: Asp185, His183 and His243 act as ligand to the iron; Arg258 and Ser260 and the Fe bind the 2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

24. (amended) A method as claimed in [any one of claims] claim 21[-23], wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.

25. (amended) A method as claimed in [any one of claims] claim 21[-23], wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.

26. (amended) A method as claimed in [any one of claims] claim 21[-23], wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

Please add the following new claims:

27. The DAOCS of claim 2, wherein said metal is iron or lead.

28. The DAOCS of claim 2, wherein said complex includes a substrate.

29. The DAOCS of claim 2, wherein said complex includes a substrate analogue.

30. The DAOCS of claim 2, wherein said complex includes an inhibitor.

31. DAOCS as claimed in claim 30, wherein the inhibitor is selected from the group consisting of N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.

32. The method of claim 8, wherein said penicillins are selected from the group consisting of penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, and penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

33. The method of claim 10, wherein said amino acid is a proteinogenic amino acid.

34. (amended) [Use as claimed in any one of claims] The method of claim 6[-8], wherein [penicillin G, penicillin V, another] unnatural substrate [or penicillin N] is converted to a [cephalosporin or] exomethylene cephalosporin.

35. The method of claim 8, wherein penicillin G, penicillin V or penicillin N is converted to a cephalosporin.

36. The method of claim 8, wherein penicillin G, penicillin V or penicillin N is converted to an exomethylene cephalosporin.

37. The enzyme of claim 12, further comprising the insertion of at least one additional amino acid residue within the region 300-311.

38. An enzyme having significant sequence similarity to DAOCS, wherein the side chain binding site of DAOC is modified and at least one additional amino acid residue is inserted within the region 300-311.

39. An enzyme having significant sequence similarity to DAOCS, wherein the side chain binding site of DAOC is modified and at least one amino acid residue at one or more of the following sites selected from the group consisting of Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, and Asn304; is changed to another amino acid residue or is deleted.

40. The enzyme of claim 12, further comprising the insertion of at least one additional amino acid residue within the region 300-311.

41. An enzyme having significant sequence similarity to DAOCS, wherein the side chain binding site of penicillin N is modified and at least one additional amino acid residue is inserted within the region 300-311.

42. The enzyme of claim 13, further comprising the insertion of at least one additional amino acid residue within the region 300-311.

43. An enzyme having significant sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of DAOC is modified and at least one additional amino acid residue is inserted within the region 300-311.

44. An enzyme having significant sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of penicillin N is modified at one or more of the following amino acid residues selected from the group consisting of Ile 88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg 306, and Arg307; is changed or deleted .

45. The enzyme of claim 13, further comprising the insertion of at least one additional amino acid residue within the region 300-311.

46. An enzyme having significant sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of DAOC is modified and at least one additional amino acid residue is inserted within the region 300-311.

47. The enzyme of claim 15, further comprising the insertion of at least one additional amino acid residue within the region 300-311.

48. An enzyme having significant sequence similarity to DAOCS, wherein both side chain and the penicillin/cephalosporin binding site of DAOC are modified and at least one additional amino acid residue is inserted within the region 300-311.

49. An enzyme according to claim 13 which is a modification of DAOCS or DACS or DAOC/DACS.

50. An enzyme according to claim 15 which is a modification of DAOCS or DACS or DAOC/DACS.

51. An enzyme as claimed in claim 13, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

52. An enzyme as claimed in claim 14, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

53. An enzyme as claimed in claim 49, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

54. An enzyme as claimed in claim 15, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

55. An enzyme as claimed in claim 37, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

56. An enzyme as claimed in claim 38, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

57. An enzyme as claimed in claim 39, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

58. An enzyme as claimed in claim 40, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

59. An enzyme as claimed in claim 41, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

60. An enzyme as claimed in claim 42, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

61. An enzyme as claimed in claim 43, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

62. An enzyme as claimed in claim 44, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

63. An enzyme as claimed in claim 45, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

64. An enzyme as claimed in claim 46, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

65. An enzyme as claimed in claim 47, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

66. An enzyme as claimed in claim 48, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

67. A polynucleotide encoding for the enzyme of claim 13.

68. A polynucleotide encoding for the enzyme of claim 14.

69. A polynucleotide encoding for the enzyme of claim 49.

70. A polynucleotide encoding for the enzyme of claim 15.

71. A polynucleotide encoding for the enzyme of claim 16.

72. A polynucleotide encoding for the enzyme of claim 37.

73. A polynucleotide encoding for the enzyme of claim 38.

74. A polynucleotide encoding for the enzyme of claim 39.

75. A polynucleotide encoding for the enzyme of claim 40.

76. A polynucleotide encoding for the enzyme of claim 41.

77. A polynucleotide encoding for the enzyme of claim 42.

78. A polynucleotide encoding for the enzyme of claim 43.

79. A polynucleotide encoding for the enzyme of claim 44.

80. A polynucleotide encoding for the enzyme of claim 45.

81. A polynucleotide encoding for the enzyme of claim 46.

82. A polynucleotide encoding for the enzyme of claim 47.

83. A polynucleotide encoding for the enzyme of claim 48.

84. A polynucleotide encoding for the enzyme of claim 50.

85. A polynucleotide encoding for the enzyme of claim 51.

86. A polynucleotide encoding for the enzyme of claim 52.

87. A polynucleotide encoding for the enzyme of claim 53.

88. A polynucleotide encoding for the enzyme of claim 54.

89. A polynucleotide encoding for the enzyme of claim 55.

90. A polynucleotide encoding for the enzyme of claim 56.

91. A polynucleotide encoding for the enzyme of claim 57.

92. A polynucleotide encoding for the enzyme of claim 58.

93. A polynucleotide encoding for the enzyme of claim 59.

94. A polynucleotide encoding for the enzyme of claim 60.

95. A polynucleotide encoding for the enzyme of claim 61.

96. A polynucleotide encoding for the enzyme of claim 62.

97. A polynucleotide encoding for the enzyme of claim 63.

98. A polynucleotide encoding for the enzyme of claim 64.

99. A micro-organism capable of expressing the polynucleotide of claim 67 under fermentation conditions.

100. A micro-organism capable of expressing the polynucleotide of claim 68 under fermentation conditions.

101. A micro-organism capable of expressing the polynucleotide of claim 69 under fermentation conditions.

102. A micro-organism capable of expressing the polynucleotide of claim 70 under fermentation conditions.

103. A micro-organism capable of expressing the polynucleotide of claim 71 under fermentation conditions.

104. A micro-organism capable of expressing the polynucleotide of claim 72 under fermentation conditions.

105. A micro-organism capable of expressing the polynucleotide of claim 73 under fermentation conditions.

106. A micro-organism capable of expressing the polynucleotide of claim 74 under fermentation conditions.

107. A micro-organism capable of expressing the polynucleotide of claim 75 under fermentation conditions.

108. A micro-organism capable of expressing the polynucleotide of claim 76 under fermentation conditions.

109. A micro-organism capable of expressing the polynucleotide of claim 77 under fermentation conditions.

110. A micro-organism capable of expressing the polynucleotide of claim 78 under fermentation conditions.

111. A micro-organism capable of expressing the polynucleotide of claim 79 under fermentation conditions.

112. A micro-organism capable of expressing the polynucleotide of claim 80 under fermentation conditions.

113. A micro-organism capable of expressing the polynucleotide of claim 81 under fermentation conditions.

114. A micro-organism capable of expressing the polynucleotide of claim 82 under fermentation conditions.

115. A micro-organism capable of expressing the polynucleotide of claim 83 under fermentation conditions.

116. A micro-organism capable of expressing the polynucleotide of claim 84 under fermentation conditions.

117. A micro-organism capable of expressing the polynucleotide of claim 85 under fermentation conditions.

118. A micro-organism capable of expressing the polynucleotide of claim 86 under fermentation conditions.

119. A micro-organism capable of expressing the polynucleotide of claim 87 under fermentation conditions.

120. A micro-organism capable of expressing the polynucleotide of claim 88 under fermentation conditions.

121. A micro-organism capable of expressing the polynucleotide of claim 89 under fermentation conditions.

122. A micro-organism capable of expressing the polynucleotide of claim 90 under fermentation conditions.

123. A micro-organism capable of expressing the polynucleotide of claim 91 under fermentation conditions.

124. A micro-organism capable of expressing the polynucleotide of claim 92 under fermentation conditions.

125. A micro-organism capable of expressing the polynucleotide of claim 93 under fermentation conditions.

126. A micro-organism capable of expressing the polynucleotide of claim 94 under fermentation conditions.

127. A micro-organism capable of expressing the polynucleotide of claim 95 under fermentation conditions.

128. A micro-organism capable of expressing the polynucleotide of claim 96 under fermentation conditions.

129. A micro-organism capable of expressing the polynucleotide of claim 97 under fermentation conditions.

130. A micro-organism capable of expressing the polynucleotide of claim 98 under fermentation conditions.

131. The method of using the micro-organisms of claim 99 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

132. The method of using the micro-organisms of claim 100 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

133. The method of using the micro-organisms of claim 101 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

134. The method of using the micro-organisms of claim 102 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

135. The method of using the micro-organisms of claim 103 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

136. The method of using the micro-organisms of claim 104 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

137. The method of using the micro-organisms of claim 105 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

138. The method of using the micro-organisms of claim 106 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

139. The method of using the micro-organisms of claim 107 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

140. The method of using the micro-organisms of claim 108 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

141. The method of using the micro-organisms of claim 109 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

142. The method of using the micro-organisms of claim 110 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

143. The method of using the micro-organisms of claim 111 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

144. The method of using the micro-organisms of claim 112 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

145. The method of using the micro-organisms of claim 113 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

146. The method of using the micro-organisms of claim 114 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

147. The method of using the micro-organisms of claim 115 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

148. The method of using the micro-organisms of claim 116 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

149. The method of using the micro-organisms of claim 117 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

150. The method of using the micro-organisms of claim 118 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

151. The method of using the micro-organisms of claim 119 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

152. The method of using the micro-organisms of claim 120 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

153. The method of using the micro-organisms of claim 121 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

154. The method of using the micro-organisms of claim 122 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

155. The method of using the micro-organisms of claim 123 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

156. The method of using the micro-organisms of claim 124 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

157. The method of using the micro-organisms of claim 125 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

158. The method of using the micro-organisms of claim 126 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

159. The method of using the micro-organisms of claim 127 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

160. The method of using the micro-organisms of claim 128 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

161. The method of using the micro-organisms of claim 129 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

162. The method of using the micro-organisms of claim 130 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

163. The method of claim 131, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

164. The method of claim 132 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

165. The method of claim 133, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

166. The method of claim 134, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

167. The method of claim 135, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

168. The method of claim 136, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

169. The method of claim 137, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

170. The method of claim 138, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

171. The method of claim 139, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

172. The method of claim 140, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

173. The method of claim 141, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

174. The method of claim 142, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

175. The method of claim 143, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

176. The method of claim 144, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

177. The method of claim 145, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

178. The method of claim 146, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

179. The method of claim 147, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

180. The method of claim 148, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

181. The method of claim 149, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

182. The method of claim 150, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

183. The method of claim 151, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

184. The method of claim 152, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

185. The method of claim 153, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

186. The method of claim 154, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

187. The method of claim 155, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

188. The method of claim 156, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

189. The method of claim 157, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

190. The method of claim 158, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

191. The method of claim 159, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

192. The method of claim 160, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

193. The method of claim 161, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

194. The method of claim 162, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

195. The method of claim 163, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

196. The method of claim 164, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

197. The method of claim 165, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

198. The method of claim 166, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

199. The method of claim 167, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

200. The method of claim 168, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

201. The method of claim 169, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

202. The method of claim 170, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

203. The method of claim 171, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

204. The method of claim 172, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

205. The method of claim 173, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

206. The method of claim 174, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

207. The method of claim 175, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

208. The method of claim 176, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

209. The method of claim 177, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

210. The method of claim 178, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

211. The method of claim 179, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

212. The method of claim 180, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

213. The method of claim 181, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

214. The method of claim 182, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

215. The method of claim 183, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

216. The method of claim 184, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

217. The method of claim 185, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

218. The method of claim 186, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

219. The method of claim 187, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

220. The method of claim 188, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

221. The method of claim 189, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

222. The method of claim 190, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

223. The method of claim 191, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

224. The method of claim 192, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

225. The method of claim 193, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

226. The method of claim 194, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

227. A method as claimed in claim 22 wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites selected from the group consisting of Thr72, Arg74, Arg75, Ile88, Glu156, Leu158, Arg160, Arg162, Phe164, Met180, Leu186, Ser187, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; Ile305, Arg 306, and Arg307; or using the following information for the design of an inhibitor: Asp185, His183 and His243 act as ligand to the iron; Arg258 and Ser260 and the Fe bind the 2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the

construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

228. A method as claimed in claim 23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.

229. A method as claimed in claim 23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.

230. A method as claimed in claim 23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

231. A polynucleotide encoding for the enzyme of claim 65.

232. A polynucleotide encoding for the enzyme of claim 66.

REMARKS

Entry of the amendments to the claims before examination of the application is respectfully requested. The claims have been amended for the sake of clarity. No new matter has been added by these amendments. Applicants authorize the Commissioner to charge any

[illegible]

Reg. No. 46,089

Date: 6-23-00
FULBRIGHT & JAWORSKI LLP
1301 McKinney, Suite 5100
Houston, Texas 77010
Phone: (713) 651-5325

MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

- 5 Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β -lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):
- 10 1. Conversion of the tripeptide: L- δ - α -aminoadipoyl-L-cysteinyl-D-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
2. In some organisms (e.g. *Penicillium chrysogenum* and
- 20 *Aspergillus nidulans*) isopenicillin N is converted by exchange of its L- δ - α -aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include
- 25 penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
3. In other organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N.
- 30 This reaction is catalysed by an epimerase enzyme.

4. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. *Streptomyces clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp.* DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are members of an extended family of Fe(II) utilising oxidase and oxygenase enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS) utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS). Since IPNS, does not use 2-oxoglutarate, it has a substantially different mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

rise to a significantly different active site.

The Invention

This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes.

Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach *et al.*, Nature, 1995, 375, 700-704; Roach *et al.*, Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens, Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

Procedures have been developed for the production of 7-aminodeacetoxycephalosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

The IPNS gene sequence (and therefore the amino acid

sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the beta-barrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach *et al.*, Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoacidipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- 5 (ii) enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. 3- β -hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes
10 that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a
15 major part of DAOCS. Previous sequence comparisons (Roach *et al.*, Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, **198**, 327). Scores over 5.0 and
20 preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, **183**, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity
25 or % similarity of amino acids possessing side chains with similar physico-chemical properties (Barton and Sternberg, J. Mol. Biol., 1987, **198**, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two
30 enzymes may have structures in which secondary structural elements are

- 6 -

largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the k_{cat}/K_m for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent k_{cat} values for penicillin N and penicillin G are similar but that K_m is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase k_{cat}/K_m for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

- 7 -

is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the β -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the α -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
- d) Glu-156. This residue binds with the α -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
- f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

- 9 -

Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

5 Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis).

10 However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

15 Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus*: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the
20 reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3 β -hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β -lactamase inhibitor,
25 clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

30 The iron-free form of DAOCS crystallises in space group R3

- 10 -

as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the
5 Fe(II)-2-oxoglutarate complex).

LEGENDS TO FIGURES.

Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

10 Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

15 Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

- 11 -

	Met Asp Thr Thr Val Pro Thr Phe Ser Leu	10
	Ala Glu Leu Gln Gln Gly Leu His Gln Asp	20
	Glu Phe Arg Arg Cys Leu Arg Asp Lys Gly	30
	Leu Phe Tyr Leu Thr Asp Cys Gly Leu Thr	40
5	Asp Thr Glu Leu Lys Ser Ala Lys Asp Leu	50
	Val Ile Asp Phe Phe Glu His Gly Ser Glu	60
	Ala Glu Lys Arg Ala Val Thr Ser Pro Val	70
	Pro Thr Met Arg Arg Gly Phe Thr Gly Leu	80
	Glu Ser Glu Ser Thr Ala Gln Ile Thr Asn	90
10	Thr Gly Ser Tyr Ser Asp Tyr Ser Met Cys	100
	Tyr Ser Met Gly Thr Ala Asp Asn Leu Phe	110
	Pro Ser Gly Asp Phe Gly Arg Ile Trp Thr	120
	Gln Tyr Phe Asp Arg Gln Tyr Thr Ala Ser	130
	Arg Ala Val Ala Arg Glu Val Leu Arg Ala	140
15	Thr Gly Thr Glu Pro Asp Gly Gly Val Glu	150
	Ala Phe Leu Asp Cys Glu Pro Leu Leu Arg	160
	Phe Arg Tyr Phe Pro Gln Val Pro Glu His	170
	Arg Ser Ala Glu Glu Gln Pro Leu Arg Met	180
	Ala Pro His Tyr Asp Leu Ser Met Val Thr	190
20	Leu Ile Gln Gln Thr Pro Cys Ala Asn Gly	200
	Phe Val Ser Leu Gln Ala Glu Val Gly Gly	210
	Ala Phe Thr Asp Leu Pro Tyr Arg Pro Asp	220
	Ala Val Leu Val Phe Cys Gly Ala Ile Ala	230
	Thr Leu Val Thr Gly Gly Gln Val Lys Ala	240
25	Pro Arg His His Val Ala Ala Pro Arg Arg	250
	Asp Gln Ile Ala Gly Ser Ser Arg Thr Ser	260
	Ser Val Phe Phe Leu Arg Pro Asn Ala Asp	270
	Phe Thr Phe Ser Val Pro Leu Ala Arg Glu	280
	Cys Gly Phe Asp Val Ser Leu Asp Gly Glu	290
30	Thr Ala Thr Phe Gln Asp Trp Ile Gly Gly	300
	Asn Tyr Val Asn Ile Arg Arg Thr Ser Lys	310
	Ala	311

- 12 -

STRUCTURE A

CRYST1	106.400	106.400	71.100	90.00	90.00	120.00
SCALE1	0.009398	0.005426	0.000000	0.000000		
SCALE2	0.000000	0.010852	0.000000	0.000000		
SCALE3	0.000000	0.000000	0.014065	0.000000		

- 13 -

ATOM	1	N	AMET	1	31.434	10.641	59.873	0.542	44.31	
ANISOU	1	N	AMET	1	8315	2319	6203	-614	-3454	-791
ATOM	2	CA	AMET	1	30.985	11.769	59.065	0.542	39.90	
ANISOU	2	CA	AMET	1	9037	3006	3117	-786	-1026	-296
ATOM	3	C	AMET	1	30.472	12.900	59.956	0.542	28.97	
ANISOU	3	C	AMET	1	4807	3113	3086	-421	-2189	-119
ATOM	4	O	AMET	1	29.961	12.670	61.055	0.542	28.12	
ANISOU	4	O	AMET	1	3925	2381	4377	-402	-1097	74
ATOM	5	CB	AMET	1	29.970	11.328	58.023	0.542	34.85	
ANISOU	5	CB	AMET	1	7877	3692	1672	30	-91	-373
ATOM	6	CG	AMET	1	28.626	12.015	57.903	0.542	38.19	
ANISOU	6	CG	AMET	1	7367	4873	2270	133	912	-1765
ATOM	7	SD	AMET	1	27.564	11.232	56.654	0.542	47.19	
ANISOU	7	SD	AMET	1	6146	7957	3827	-2344	1050	-1326
ATOM	8	CE	AMET	1	28.129	11.973	55.135	0.542	27.10	
ANISOU	8	CE	AMET	1	5030	2111	3155	2345	-1467	-9
ATOM	9	N	AASP	2	30.592	14.105	59.425	0.268	30.20	
ANISOU	9	N	AASP	2	4674	3022	3777	-1210	-782	-383
ATOM	10	CA	AASP	2	29.993	15.322	59.963	0.268	34.22	
ANISOU	10	CA	AASP	2	5567	2803	4633	-1106	-964	-525
ATOM	11	C	AASP	2	28.494	15.268	59.655	0.268	33.34	
ANISOU	11	C	AASP	2	5665	1997	5006	-314	-1457	877
ATOM	12	O	AASP	2	28.099	15.650	58.551	0.268	44.76	
ANISOU	12	O	AASP	2	6859	5248	4901	-1023	-1582	1631
ATOM	13	CB	AASP	2	30.629	16.528	59.281	0.268	25.98	
ANISOU	13	CB	AASP	2	4424	3085	2361	322	-1794	582
ATOM	14	CG	AASP	2	29.978	17.862	59.553	0.268	38.05	
ANISOU	14	CG	AASP	2	6456	2611	5389	-501	-608	-1114
ATOM	15	OD1	AASP	2	28.995	17.937	60.318	0.268	42.35	
ANISOU	15	OD1	AASP	2	6406	504	9179	873	920	1991
ATOM	16	OD2	AASP	2	30.449	18.885	58.997	0.268	28.59	
ANISOU	16	OD2	AASP	2	1619	2901	6341	790	-1022	-253
ATOM	17	N	BMET	1	32.709	12.640	58.544	0.458	29.49	
ANISOU	17	N	BMET	1	4552	2218	4435	-105	1580	477
ATOM	18	CA	BMET	1	31.874	13.050	57.425	0.458	40.62	
ANISOU	18	CA	BMET	1	4228	4809	6395	580	210	103
ATOM	19	C	BMET	1	30.884	14.113	57.894	0.458	38.21	
ANISOU	19	C	BMET	1	5082	3637	5797	282	-909	-915
ATOM	20	O	BMET	1	30.075	14.599	57.110	0.458	44.81	
ANISOU	20	O	BMET	1	8292	3208	5525	2071	-656	-12
ATOM	21	CB	BMET	1	31.131	11.857	56.829	0.458	33.14	
ANISOU	21	CB	BMET	1	4866	2613	5114	2013	-122	818
ATOM	22	CG	BMET	1	29.625	11.840	56.968	0.458	40.28	
ANISOU	22	CG	BMET	1	4795	5740	4768	230	-751	53
ATOM	23	SD	BMET	1	28.761	11.495	55.422	0.458	34.23	
ANISOU	23	SD	BMET	1	5619	3819	3566	2050	-215	20
ATOM	24	CE	BMET	1	29.953	12.079	54.222	0.458	54.24	
ANISOU	24	CE	BMET	1	10672	4519	5420	1149	4083	-2463
ATOM	25	N	BASP	2	30.914	14.381	59.194	0.732	37.72	
ANISOU	25	N	BASP	2	4433	3914	5984	-1323	-1208	-1385
ATOM	26	CA	BASP	2	29.979	15.308	59.811	0.732	35.78	
ANISOU	26	CA	BASP	2	5412	3387	4794	-1064	-1050	-795
ATOM	27	C	BASP	2	28.536	14.886	59.567	0.732	29.66	
ANISOU	27	C	BASP	2	4876	1624	4771	27	-1561	1218
ATOM	28	O	BASP	2	28.181	14.602	58.414	0.732	34.65	
ANISOU	28	O	BASP	2	4375	3689	5100	65	-1485	247
ATOM	29	CB	BASP	2	30.195	16.696	59.181	0.732	37.39	
ANISOU	29	CB	BASP	2	6632	3351	4222	-1850	869	-1518
ATOM	30	CG	BASP	2	29.562	17.730	60.104	0.732	30.38	
ANISOU	30	CG	BASP	2	3243	3791	4510	-500	-606	-1191
ATOM	31	OD1	BASP	2	28.866	17.247	61.030	0.732	48.88	

- 14 -

ANISOU	31	OD1	BASP	2	6276	4203	8095	-1203	3147	-1901
ATOM	32	OD2	BASP	2	29.760	18.945	59.875	0.732	34.85	
ANISOU	32	OD2	BASP	2	2852	3708	6680	-491	444	-1450
ATOM	33	N	THR	3	27.717	14.789	60.606	1.000	35.58	
ANISOU	33	N	THR	3	4586	4123	4811	601	-1628	1516
ATOM	34	CA	THR	3	26.303	14.433	60.495	1.000	40.48	
ANISOU	34	CA	THR	3	4650	4555	6175	371	-911	-385
ATOM	35	C	THR	3	25.382	15.647	60.611	1.000	39.82	
ANISOU	35	C	THR	3	4376	4155	6598	320	-3864	-586
ATOM	36	O	THR	3	24.150	15.556	60.751	1.000	33.55	
ANISOU	36	O	THR	3	4668	3107	4972	357	-2748	-588
ATOM	37	CB	THR	3	25.905	13.450	61.613	1.000	39.95	
ANISOU	37	CB	THR	3	3787	4004	7387	160	-1209	62
ATOM	38	OG1	THR	3	26.591	13.851	62.817	1.000	61.83	
ANISOU	38	OG1	THR	3	10134	5882	7476	-4164	-3020	2051
ATOM	39	CG2	THR	3	26.399	12.052	61.278	1.000	59.32	
ANISOU	39	CG2	THR	3	4613	3971	13955	1114	-3135	-198
ATOM	40	N	THR	4	26.036	16.780	60.456	1.000	32.55	
ANISOU	40	N	THR	4	4306	4611	3450	377	-2166	-217
ATOM	41	CA	THR	4	25.439	18.092	60.393	1.000	31.22	
ANISOU	41	CA	THR	4	4275	4229	3358	-81	-1179	95
ATOM	42	C	THR	4	24.672	18.272	59.090	1.000	30.06	
ANISOU	42	C	THR	4	4876	3341	3207	773	-1156	-204
ATOM	43	O	THR	4	25.195	17.935	58.017	1.000	31.64	
ANISOU	43	O	THR	4	4877	3780	3363	1935	-1255	-52
ATOM	44	CB	THR	4	26.510	19.208	60.407	1.000	32.31	
ANISOU	44	CB	THR	4	2320	4762	5194	475	-547	593
ATOM	45	OG1	THR	4	27.324	19.091	61.578	1.000	32.36	
ANISOU	45	OG1	THR	4	3705	3955	4635	-79	-797	-389
ATOM	46	CG2	THR	4	25.852	20.582	60.458	1.000	27.22	
ANISOU	46	CG2	THR	4	3728	4174	2443	71	304	-151
ATOM	47	N	VAL	5	23.464	18.796	59.211	1.000	21.69	
ANISOU	47	N	VAL	5	4041	1985	2215	-543	-657	158
ATOM	48	CA	VAL	5	22.690	19.140	58.024	1.000	20.42	
ANISOU	48	CA	VAL	5	3675	1964	2120	-622	-517	103
ATOM	49	C	VAL	5	23.199	20.489	57.499	1.000	17.01	
ANISOU	49	C	VAL	5	2263	1803	2396	-279	-622	89
ATOM	50	O	VAL	5	23.156	21.449	58.252	1.000	21.10	
ANISOU	50	O	VAL	5	3662	1885	2472	-389	-656	16
ATOM	51	CB	VAL	5	21.204	19.216	58.402	1.000	24.22	
ANISOU	51	CB	VAL	5	3551	2155	3495	-1045	-396	783
ATOM	52	CG1	VAL	5	20.434	19.700	57.166	1.000	20.14	
ANISOU	52	CG1	VAL	5	3202	1779	2672	-453	10	-226
ATOM	53	CG2	VAL	5	20.701	17.867	58.860	1.000	28.58	
ANISOU	53	CG2	VAL	5	5258	2086	3516	-1226	431	510
ATOM	54	N	PRO	6	23.750	20.542	56.300	1.000	16.95	
ANISOU	54	N	PRO	6	2378	1629	2434	29	-594	301
ATOM	55	CA	PRO	6	24.354	21.793	55.857	1.000	16.90	
ANISOU	55	CA	PRO	6	1645	1775	3000	6	-445	303
ATOM	56	C	PRO	6	23.298	22.800	55.383	1.000	15.61	
ANISOU	56	C	PRO	6	1477	1766	2687	-192	-437	545
ATOM	57	O	PRO	6	22.133	22.432	55.201	1.000	15.75	
ANISOU	57	O	PRO	6	1578	1761	2647	-260	-579	55
ATOM	58	CB	PRO	6	25.216	21.375	54.682	1.000	19.85	
ANISOU	58	CB	PRO	6	2320	1752	3468	50	70	182
ATOM	59	CG	PRO	6	24.632	20.095	54.187	1.000	24.76	
ANISOU	59	CG	PRO	6	3550	2953	2904	-1186	300	-286
ATOM	60	CD	PRO	6	23.926	19.428	55.357	1.000	17.91	
ANISOU	60	CD	PRO	6	1960	1962	2882	-168	-138	-44
ATOM	61	N	THR	7	23.723	24.031	55.156	1.000	14.38	
ANISOU	61	N	THR	7	1518	1567	2378	-158	-616	100

- 15 -

ATOM	62	CA	THR	7	22.907	25.103	54.610	1.000	14.09
ANISOU	62	CA	THR	7	1625	1554	2174	-255	-581 2 2 8
ATOM	63	C	THR	7	23.605	25.684	53.374	1.000	14.74
ANISOU	63	C	THR	7	1683	1849	2067	-193	-468 1 2 1
ATOM	64	O	THR	7	24.828	25.894	53.423	1.000	15.95
ANISOU	64	O	THR	7	1752	2137	2171	-378	-457 1 8 5
ATOM	65	CB	THR	7	22.795	26.248	55.637	1.000	15.25
ANISOU	65	CB	THR	7	1548	1846	2401	56	-124 5 2
ATOM	66	OG1	THR	7	22.208	25.717	56.829	1.000	16.91
ANISOU	66	OG1	THR	7	1818	2149	2458	-402	-183 4 7
ATOM	67	CG2	THR	7	21.952	27.387	55.040	1.000	16.09
ANISOU	67	CG2	THR	7	1651	1613	2848	-138	-263 - 2 5
ATOM	68	N	PHE	8	22.830	25.892	52.325	1.000	15.06
ANISOU	68	N	PHE	8	1966	1618	2137	-411	-558 2 3 0
ATOM	69	CA	PHE	8	23.317	26.545	51.136	1.000	14.76
ANISOU	69	CA	PHE	8	1857	1558	2192	-213	-411 2 8 1
ATOM	70	C	PHE	8	22.421	27.728	50.810	1.000	14.94
ANISOU	70	C	PHE	8	1907	1421	2347	-275	-357 1 8 1
ATOM	71	O	PHE	8	21.198	27.678	50.995	1.000	16.40
ANISOU	71	O	PHE	8	1782	1642	2808	-197	-550 3 4
ATOM	72	CB	PHE	8	23.242	25.562	49.948	1.000	16.49
ANISOU	72	CB	PHE	8	2123	1854	2287	49	-371 - 1
ATOM	73	CG	PHE	8	24.225	24.432	50.027	1.000	14.92
ANISOU	73	CG	PHE	8	1710	1824	2135	-197	-365 1 6 3
ATOM	74	CD1	PHE	8	23.822	23.227	50.600	1.000	16.78
ANISOU	74	CD1	PHE	8	1808	1726	2842	-300	-358 1 8 4
ATOM	75	CD2	PHE	8	25.539	24.558	49.602	1.000	16.67
ANISOU	75	CD2	PHE	8	1705	2130	2500	-310	-361 3 2 1
ATOM	76	CE1	PHE	8	24.702	22.183	50.742	1.000	16.74
ANISOU	76	CE1	PHE	8	2035	1966	2359	-4	-99 2 9 5
ATOM	77	CE2	PHE	8	26.420	23.525	49.773	1.000	19.18
ANISOU	77	CE2	PHE	8	1398	2153	3736	-408	-631 1 8 7
ATOM	78	CZ	PHE	8	26.026	22.336	50.351	1.000	17.90
ANISOU	78	CZ	PHE	8	1849	2003	2948	-119	-376 2 0
ATOM	79	N	SER	9	23.023	28.776	50.314	1.000	14.82
ANISOU	79	N	SER	9	2134	1488	2008	-351	-528 3 1 0
ATOM	80	CA	SER	9	22.338	29.902	49.715	1.000	15.12
ANISOU	80	CA	SER	9	2037	1259	2449	-357	-571 1 3 4
ATOM	81	C	SER	9	21.977	29.607	48.270	1.000	16.19
ANISOU	81	C	SER	9	2138	1791	2224	-374	-535 5 4 7
ATOM	82	O	SER	9	22.877	29.312	47.473	1.000	17.04
ANISOU	82	O	SER	9	2191	1892	2393	-423	-544 2 3 2
ATOM	83	CB	SER	9	23.306	31.113	49.696	1.000	18.74
ANISOU	83	CB	SER	9	2891	1712	2519	-1012	-478 7 1 7
ATOM	84	OG	SER	9	22.738	32.131	48.853	1.000	20.82
ANISOU	84	OG	SER	9	2866	1569	3477	-662	-854 6 0 7
ATOM	85	N	LEU	10	20.697	29.674	47.924	1.000	16.46
ANISOU	85	N	LEU	10	2215	1495	2542	-228	-740 - 4 8
ATOM	86	CA	LEU	10	20.345	29.401	46.529	1.000	17.55
ANISOU	86	CA	LEU	10	2263	1856	2551	-582	-694 3 6
ATOM	87	C	LEU	10	21.079	30.373	45.591	1.000	18.84
ANISOU	87	C	LEU	10	2506	1870	2784	-596	-830 3 5 7
ATOM	88	O	LEU	10	21.573	30.025	44.520	1.000	20.19
ANISOU	88	O	LEU	10	2705	2263	2704	-524	-663 5 0 8
ATOM	89	CB	LEU	10	18.844	29.559	46.327	1.000	18.87
ANISOU	89	CB	LEU	10	2302	2516	2354	-288	-715 2 8 0
ATOM	90	CG	LEU	10	18.355	29.333	44.895	1.000	18.28
ANISOU	90	CG	LEU	10	2182	2172	2591	-668	-677 - 3 0 1
ATOM	91	CD1	LEU	10	18.708	27.955	44.397	1.000	22.45
ANISOU	91	CD1	LEU	10	3418	2024	3089	-308	-537 1 7
ATOM	92	CD2	LEU	10	16.852	29.603	44.869	1.000	21.93

- 16 -

ANISOU	92	CD2	LEU	10	2250	2658	3424	-504	-1139	7	5
ATOM	93	N	ALA	11	21.154	31.638	46.037	1.000	20.05		
ANISOU	93	N	ALA	11	2862	1780	2977	-595	-1279	4	7
ATOM	94	CA	ALA	11	21.810	32.647	45.202	1.000	24.24		
ANISOU	94	CA	ALA	11	3160	1670	4380	-455	-979	8	9
ATOM	95	C	ALA	11	23.285	32.309	44.946	1.000	21.06		
ANISOU	95	C	ALA	11	3128	1937	2937	-644	-1016	4	3
ATOM	96	O	ALA	11	23.819	32.447	43.829	1.000	26.29		
ANISOU	96	O	ALA	11	3569	3261	3158	-1628	-923	1	1
ATOM	97	CB	ALA	11	21.752	33.989	45.953	1.000	24.29		
ANISOU	97	CB	ALA	11	3740	1692	3797	-461	-216	9	9
ATOM	98	N	GLU	12	23.953	31.844	46.005	1.000	20.65		
ANISOU	98	N	GLU	12	2829	1975	3044	-828	-930	6	7
ATOM	99	CA	GLU	12	25.354	31.463	45.862	1.000	21.19		
ANISOU	99	CA	GLU	12	3036	2400	2615	-506	-715	5	9
ATOM	100	C	GLU	12	25.483	30.277	44.920	1.000	21.56		
ANISOU	100	C	GLU	12	3894	2179	2117	-702	-206	9	8
ATOM	101	O	GLU	12	26.375	30.215	44.069	1.000	21.98		
ANISOU	101	O	GLU	12	3463	2917	1971	-1144	-488	6	1
ATOM	102	CB	GLU	12	26.032	31.170	47.204	1.000	20.27		
ANISOU	102	CB	GLU	12	2874	2192	2636	-221	-624	5	0
ATOM	103	CG	GLU	12	26.156	32.451	48.032	1.000	20.54		
ANISOU	103	CG	GLU	12	2889	2316	2598	-344	-516	4	0
ATOM	104	CD	GLU	12	26.787	32.279	49.389	1.000	21.86		
ANISOU	104	CD	GLU	12	3146	2542	2619	-1297	-612	7	9
ATOM	105	OE1	GLU	12	27.068	31.149	49.803	1.000	24.98		
ANISOU	105	OE1	GLU	12	3642	2681	3169	-1348	-1088	1	1
ATOM	106	OE2	GLU	12	26.819	33.305	50.092	1.000	33.52		
ANISOU	106	OE2	GLU	12	5881	2966	3888	-1119	-2251	4	6
ATOM	107	N	LEU	13	24.600	29.295	45.060	1.000	18.91		
ANISOU	107	N	LEU	13	2567	2345	2275	-351	-390	3	8
ATOM	108	CA	LEU	13	24.645	28.117	44.174	1.000	18.61		
ANISOU	108	CA	LEU	13	2575	2347	2149	-209	270	4	0
ATOM	109	C	LEU	13	24.432	28.566	42.738	1.000	21.40		
ANISOU	109	C	LEU	13	3558	2367	2206	-709	-41	5	2
ATOM	110	O	LEU	13	25.102	28.095	41.824	1.000	23.75		
ANISOU	110	O	LEU	13	3827	3216	1981	-823	-117	1	9
ATOM	111	CB	LEU	13	23.541	27.137	44.562	1.000	18.97		
ANISOU	111	CB	LEU	13	2982	2243	1984	-462	-145	4	4
ATOM	112	CG	LEU	13	23.773	26.344	45.860	1.000	18.57		
ANISOU	112	CG	LEU	13	2313	2322	2422	-467	-362	7	4
ATOM	113	CD1	LEU	13	22.526	25.480	46.070	1.000	20.74		
ANISOU	113	CD1	LEU	13	2769	2266	2845	-789	-142	5	9
ATOM	114	CD2	LEU	13	25.023	25.473	45.858	1.000	19.80		
ANISOU	114	CD2	LEU	13	2709	2229	2585	-244	-509	-1	0
ATOM	115	N	GLN	14	23.544	29.508	42.478	1.000	22.03		
ANISOU	115	N	GLN	14	3596	2139	2635	-960	-903	3	7
ATOM	116	CA	GLN	14	23.284	29.978	41.104	1.000	23.79		
ANISOU	116	CA	GLN	14	3010	3335	2694	-992	-816	6	4
ATOM	117	C	GLN	14	24.481	30.712	40.509	1.000	25.44		
ANISOU	117	C	GLN	14	3360	3427	2881	-1070	-382	4	8
ATOM	118	O	GLN	14	24.655	30.829	39.288	1.000	30.04		
ANISOU	118	O	GLN	14	3836	4657	2922	-1208	-427	8	9
ATOM	119	CB	GLN	14	22.064	30.906	41.131	1.000	26.28		
ANISOU	119	CB	GLN	14	3133	3630	3222	-760	-863	9	3
ATOM	120	CG	GLN	14	20.772	30.111	41.355	1.000	23.26		
ANISOU	120	CG	GLN	14	3106	2319	3413	-299	-577	5	1
ATOM	121	CD	GLN	14	19.586	31.020	41.631	1.000	23.69		
ANISOU	121	CD	GLN	14	3384	2462	3155	-317	-393	-1	9
ATOM	122	OE1	GLN	14	19.734	32.104	42.160	1.000	28.34		
ANISOU	122	OE1	GLN	14	4973	2619	3175	-183	-732	-4	0

- 17 -

ATOM	123	NE2	GLN	14	18.398	30.513	41.349	1.000	23.60
ANISOU	123	NE2	GLN	14	3058	2969	2941	-383	54 2 4 5
ATOM	124	N	GLN	15	25.309	31.243	41.395	1.000	25.00
ANISOU	124	N	GLN	15	3078	3281	3140	-1159	-394 5 7 5
ATOM	125	CA	GLN	15	26.530	31.936	40.945	1.000	24.05
ANISOU	125	CA	GLN	15	2947	3560	2631	-866	-98 6 5 5
ATOM	126	C	GLN	15	27.650	30.920	40.707	1.000	26.06
ANISOU	126	C	GLN	15	3810	3951	2139	-345	406 6 6 8
ATOM	127	O	GLN	15	28.756	31.284	40.302	1.000	35.85
ANISOU	127	O	GLN	15	4294	4851	4476	102	1871 1 1 9 2
ATOM	128	CB	GLN	15	27.018	32.918	42.009	1.000	25.90
ANISOU	128	CB	GLN	15	3055	3037	3748	-1092	-109 3 6 4
ATOM	129	CG	GLN	15	26.103	34.092	42.219	1.000	31.24
ANISOU	129	CG	GLN	15	4562	2577	4731	-806	962 1 0 5 4
ATOM	130	CD	GLN	15	26.503	35.022	43.348	1.000	59.75
ANISOU	130	CD	GLN	15	9927	2475	10301	-1855	-14 -190 4
ATOM	131	OE1	GLN	15	27.634	35.031	43.840	1.000	81.81
ANISOU	131	OE1	GLN	15	15059	3931	12094	-944	-6272 -180 3
ATOM	132	NE2	GLN	15	25.539	35.841	43.767	1.000	91.46
ANISOU	132	NE2	GLN	15	14070	4846	15833	-923	3672 -485 0
ATOM	133	N	GLY	16	27.379	29.643	40.969	1.000	29.90
ANISOU	133	N	GLY	16	4634	3820	2907	-239	22 7 8 7
ATOM	134	CA	GLY	16	28.410	28.649	40.699	1.000	28.76
ANISOU	134	CA	GLY	16	4466	3629	2833	-709	461 2 5 0
ATOM	135	C	GLY	16	29.339	28.473	41.878	1.000	27.60
ANISOU	135	C	GLY	16	3816	3779	2891	-616	914 1 4 8 5
ATOM	136	O	GLY	16	30.398	27.867	41.725	1.000	31.47
ANISOU	136	O	GLY	16	3386	4758	3814	-899	1243 1 0 2 3
ATOM	137	N	LEU	17	28.960	28.898	43.083	1.000	26.01
ANISOU	137	N	LEU	17	3295	3636	2950	-721	162 7 4 3
ATOM	138	CA	LEU	17	29.776	28.666	44.257	1.000	23.96
ANISOU	138	CA	LEU	17	2700	3032	3372	-601	100 6 7 3
ATOM	139	C	LEU	17	29.462	27.338	44.932	1.000	20.31
ANISOU	139	C	LEU	17	2222	2763	2733	-252	611 2 6 1
ATOM	140	O	LEU	17	28.389	26.780	44.789	1.000	23.13
ANISOU	140	O	LEU	17	2347	3134	3308	-443	263 8 5 9
ATOM	141	CB	LEU	17	29.645	29.806	45.286	1.000	25.94
ANISOU	141	CB	LEU	17	2886	2933	4035	-1318	-405 2 5 4
ATOM	142	CG	LEU	17	29.962	31.209	44.716	1.000	31.57
ANISOU	142	CG	LEU	17	3741	2948	5308	-523	1150 7 2 2
ATOM	143	CD1	LEU	17	29.550	32.358	45.615	1.000	32.04
ANISOU	143	CD1	LEU	17	5221	2887	4066	-1269	278 5 0 8
ATOM	144	CD2	LEU	17	31.458	31.278	44.416	1.000	38.11
ANISOU	144	CD2	LEU	17	3828	5491	5160	-2315	954 2 3 2
ATOM	145	N	HIS	18	30.441	26.822	45.681	1.000	22.49
ANISOU	145	N	HIS	18	2600	3067	2877	-662	42 4 4 9
ATOM	146	CA	HIS	18	30.289	25.644	46.537	1.000	21.54
ANISOU	146	CA	HIS	18	2378	2809	2996	-432	201 3 1 3
ATOM	147	C	HIS	18	29.908	24.376	45.790	1.000	22.76
ANISOU	147	C	HIS	18	2256	3245	3148	-1009	282 1 1 4
ATOM	148	O	HIS	18	29.147	23.565	46.331	1.000	22.60
ANISOU	148	O	HIS	18	2008	3064	3516	-629	-166 8 8 4
ATOM	149	CB	HIS	18	29.224	25.872	47.618	1.000	22.81
ANISOU	149	CB	HIS	18	2514	2879	3272	-526	450 4 2 1
ATOM	150	CG	HIS	18	29.320	27.248	48.217	1.000	21.70
ANISOU	150	CG	HIS	18	2797	3038	2411	-149	39 5 0 3
ATOM	151	ND1	HIS	18	30.438	27.773	48.807	1.000	25.01
ANISOU	151	ND1	HIS	18	3714	3505	2284	-207	-629 1 4 9
ATOM	152	CD2	HIS	18	28.370	28.216	48.269	1.000	24.95
ANISOU	152	CD2	HIS	18	3244	3278	2957	87 544	2 7 5
ATOM	153	CE1	HIS	18	30.197	28.982	49.223	1.000	29.26

- 18 -

ANISOU 153 CE1 HIS 18 4603 3396 3118 -388 -335 2 7
 ATOM 154 NE2 HIS 18 28.937 29.271 48.919 1.000 27.24
 ANISOU 154 NE2 HIS 18 4582 3137 2632 2 224 3 6 5
 ATOM 155 N GLN 19 30.269 24.270 44.521 1.000 22.74
 ANISOU 155 N GLN 19 2724 3094 2822 -511 -123 4 2 3
 ATOM 156 CA GLN 19 29.806 23.113 43.730 1.000 23.85
 ANISOU 156 CA GLN 19 3129 2668 3263 148 63 8 9
 ATOM 157 C GLN 19 30.271 21.760 44.221 1.000 22.77
 ANISOU 157 C GLN 19 2532 3026 3095 -502 -574 7 7 8
 ATOM 158 O GLN 19 29.480 20.801 44.259 1.000 21.99
 ANISOU 158 O GLN 19 1869 2911 3574 -187 0 5 5 8
 ATOM 159 CB GLN 19 30.227 23.322 42.276 1.000 27.66
 ANISOU 159 CB GLN 19 5043 2519 2947 29 -339 4 5 8
 ATOM 160 CG GLN 19 29.397 24.333 41.523 1.000 26.21
 ANISOU 160 CG GLN 19 3289 3163 3508 299 171 4 3 7
 ATOM 161 CD GLN 19 27.917 24.368 41.862 1.000 32.47
 ANISOU 161 CD GLN 19 3403 4411 4521 -986 535 6 5 4
 ATOM 162 OE1 GLN 19 27.154 23.604 41.277 1.000 39.69
 ANISOU 162 OE1 GLN 19 3996 4238 6845 -262 -2770 18 2 9
 ATOM 163 NE2 GLN 19 27.511 25.212 42.811 1.000 42.55
 ANISOU 163 NE2 GLN 19 3803 6153 6212 81 1944 1 1
 ATOM 164 N ASP 20 31.526 21.572 44.631 1.000 22.63
 ANISOU 164 N ASP 20 2073 3400 3123 -414 95 7 0 8
 ATOM 165 CA ASP 20 31.926 20.292 45.225 1.000 23.10
 ANISOU 165 CA ASP 20 1869 3674 3235 83 236 7 0 4
 ATOM 166 C ASP 20 31.190 20.042 46.546 1.000 20.03
 ANISOU 166 C ASP 20 1775 2963 2873 -280 -143 4 9 3
 ATOM 167 O ASP 20 30.772 18.899 46.768 1.000 21.48
 ANISOU 167 O ASP 20 1429 2884 3848 -311 225 2 2 4
 ATOM 168 CB ASP 20 33.414 20.268 45.521 1.000 27.66
 ANISOU 168 CB ASP 20 1835 4546 4130 -16 207 8 8 1
 ATOM 169 CG ASP 20 34.298 20.206 44.291 1.000 39.35
 ANISOU 169 CG ASP 20 2355 6893 5705 -654 1323 -19 1 5
 ATOM 170 OD1 ASP 20 33.870 19.914 43.153 1.000 35.78
 ANISOU 170 OD1 ASP 20 3152 5452 4992 -741 1508 -7 9 7
 ATOM 171 OD2 ASP 20 35.508 20.433 44.467 1.000 45.22
 ANISOU 171 OD2 ASP 20 2201 8705 6277 -589 1088 -8 7
 ATOM 172 N GLU 21 31.046 21.053 47.404 1.000 20.01
 ANISOU 172 N GLU 21 1574 2935 3093 -412 -241 3 6 7
 ATOM 173 CA GLU 21 30.323 20.811 48.665 1.000 18.97
 ANISOU 173 CA GLU 21 1412 2956 2838 -481 -464 1 1 8
 ATOM 174 C GLU 21 28.858 20.448 48.402 1.000 17.84
 ANISOU 174 C GLU 21 1386 2342 3050 -307 -395 2 3 4
 ATOM 175 O GLU 21 28.290 19.602 49.054 1.000 18.46
 ANISOU 175 O GLU 21 1671 2286 3057 -419 -351 1 1 6
 ATOM 176 CB GLU 21 30.415 22.058 49.563 1.000 20.10
 ANISOU 176 CB GLU 21 1646 2821 3170 -514 -499 1 2 7
 ATOM 177 CG GLU 21 31.893 22.322 49.918 1.000 24.11
 ANISOU 177 CG GLU 21 1682 3568 3912 -766 -326 -7 1 1
 ATOM 178 CD GLU 21 32.574 23.380 49.081 1.000 29.70
 ANISOU 178 CD GLU 21 1330 4241 5713 -752 -666 5 2 1
 ATOM 179 OE1 GLU 21 32.249 23.594 47.887 1.000 35.14
 ANISOU 179 OE1 GLU 21 2623 4054 6677 -1336 -1741 19 7 7
 ATOM 180 OE2 GLU 21 33.483 24.007 49.678 1.000 39.39
 ANISOU 180 OE2 GLU 21 3681 4425 6860 -2089 -1618 6 4 7
 ATOM 181 N PHE 22 28.231 21.048 47.395 1.000 17.30
 ANISOU 181 N PHE 22 1540 2352 2680 -243 -446 -7 9
 ATOM 182 CA PHE 22 26.851 20.761 47.071 1.000 17.13
 ANISOU 182 CA PHE 22 1534 2166 2807 -235 -396 3 7 4
 ATOM 183 C PHE 22 26.733 19.329 46.552 1.000 17.41
 ANISOU 183 C PHE 22 1688 2500 2427 -502 -334 1 0 4

- 19 -

ATOM	184	O	PHE	22	25.867	18.574	46.995	1.000	15.87
ANISOU	184	O	PHE	22	1570	2118	2343	-249	-361 1 3 1
ATOM	185	CB	PHE	22	26.305	21.840	46.149	1.000	18.00
ANISOU	185	CB	PHE	22	1747	2754	2337	70	-178 4 4 5
ATOM	186	CG	PHE	22	24.802	21.729	45.930	1.000	16.38
ANISOU	186	CG	PHE	22	1763	1748	2714	-90	-326 2 2 3
ATOM	187	CD1	PHE	22	23.934	21.723	47.003	1.000	18.29
ANISOU	187	CD1	PHE	22	1812	2091	3045	-197	-88 5 7 6
ATOM	188	CD2	PHE	22	24.290	21.720	44.641	1.000	18.62
ANISOU	188	CD2	PHE	22	2106	2079	2890	-143	-623 3 9 4
ATOM	189	CE1	PHE	22	22.569	21.727	46.771	1.000	18.90
ANISOU	189	CE1	PHE	22	1826	2086	3271	-198	-133 3 0 2
ATOM	190	CE2	PHE	22	22.911	21.660	44.379	1.000	19.28
ANISOU	190	CE2	PHE	22	2189	2023	3114	-242	-754 -1 4 4
ATOM	191	CZ	PHE	22	22.059	21.645	45.473	1.000	19.42
ANISOU	191	CZ	PHE	22	2048	1723	3607	90	-483 -3 7 6
ATOM	192	N	ARG	23	27.580	18.971	45.583	1.000	17.88
ANISOU	192	N	ARG	23	1647	2437	2709	-168	-218 3 1 7
ATOM	193	CA	ARG	23	27.520	17.594	45.079	1.000	19.18
ANISOU	193	CA	ARG	23	1724	2539	3022	-166	36 1 5 8
ATOM	194	C	ARG	23	27.767	16.595	46.211	1.000	19.11
ANISOU	194	C	ARG	23	1279	2461	3518	-173	-113 4 5 5
ATOM	195	O	ARG	23	27.107	15.547	46.229	1.000	18.82
ANISOU	195	O	ARG	23	1614	2156	3381	-33	181 -1 2 8
ATOM	196	CB	ARG	23	28.605	17.351	44.030	1.000	22.81
ANISOU	196	CB	ARG	23	1934	4099	2633	-34	-105 -3 5 4
ATOM	197	CG	ARG	23	28.248	17.790	42.617	1.000	24.82
ANISOU	197	CG	ARG	23	2601	4078	2752	191	-122 -2 0 4
ATOM	198	CD	ARG	23	29.376	17.272	41.685	1.000	29.71
ANISOU	198	CD	ARG	23	2503	5619	3168	-285	908 7 0 4
ATOM	199	NE	ARG	23	30.479	18.206	41.800	1.000	30.96
ANISOU	199	NE	ARG	23	2877	5034	3851	-43	286 2 9 7
ATOM	200	CZ	ARG	23	30.549	19.360	41.148	1.000	29.49
ANISOU	200	CZ	ARG	23	2612	5063	3529	-225	606 1 7 7
ATOM	201	NH1	ARG	23	29.536	19.665	40.328	1.000	29.26
ANISOU	201	NH1	ARG	23	3242	4951	2923	-960	331 5 2 5
ATOM	202	NH2	ARG	23	31.629	20.092	41.345	1.000	32.61
ANISOU	202	NH2	ARG	23	2320	5347	4722	-134	519 1 7 9
ATOM	203	N	ARG	24	28.708	16.851	47.125	1.000	17.80
ANISOU	203	N	ARG	24	1262	2168	3332	183	38 9 8
ATOM	204	CA	ARG	24	28.930	15.899	48.222	1.000	18.85
ANISOU	204	CA	ARG	24	1368	2509	3287	69	-162 1 0 5
ATOM	205	C	ARG	24	27.701	15.811	49.114	1.000	17.51
ANISOU	205	C	ARG	24	1456	2015	3181	132	-177 2 4 3
ATOM	206	O	ARG	24	27.333	14.733	49.544	1.000	17.93
ANISOU	206	O	ARG	24	1851	1965	2997	-16	-402 2 5 3
ATOM	207	CB	ARG	24	30.203	16.321	48.991	1.000	19.88
ANISOU	207	CB	ARG	24	1685	2700	3169	-398	-218 4 4
ATOM	208	CG	ARG	24	31.459	16.053	48.135	1.000	29.07
ANISOU	208	CG	ARG	24	1467	4625	4954	269	203 7 0 9
ATOM	209	CD	ARG	24	32.700	16.206	49.016	1.000	41.84
ANISOU	209	CD	ARG	24	1745	7021	7130	-451	-494 -9 2 2
ATOM	210	NE	ARG	24	33.690	17.103	48.464	1.000	57.06
ANISOU	210	NE	ARG	24	4362	9316	8003	-3326	-669 -11 4 1
ATOM	211	CZ	ARG	24	34.032	18.327	48.810	1.000	60.67
ANISOU	211	CZ	ARG	24	5961	10369	6723	-4627	-1324 -1 5 8 6
ATOM	212	NH1	ARG	24	33.430	18.980	49.799	1.000	49.70
ANISOU	212	NH1	ARG	24	7748	6565	4569	-951	-2185 2 2 2 6
ATOM	213	NH2	ARG	24	34.997	18.971	48.159	1.000	54.12
ANISOU	213	NH2	ARG	24	8696	8490	3378	-3780	-2352 1 6 0 7
ATOM	214	N	CYS	25	27.092	16.963	49.370	1.000	15.74

- 20 -

ANISOU	214	N	CYS	25	1435	1969	2574	-16	-393	- 3 3
ATOM	215	CA	CYS	25	25.884	16.921	50.223	1.000	16.39	
ANISOU	215	CA	CYS	25	1518	1954	2756	-95	-317	- 3 0 0
ATOM	216	C	CYS	25	24.826	16.068	49.547	1.000	15.73	
ANISOU	216	C	CYS	25	1629	1699	2648	-114	-432	6 6
ATOM	217	O	CYS	25	24.124	15.262	50.155	1.000	15.89	
ANISOU	217	O	CYS	25	1453	1801	2783	-88	-469	2 5 2
ATOM	218	CB	CYS	25	25.367	18.362	50.424	1.000	15.93	
ANISOU	218	CB	CYS	25	1644	1779	2629	-49	-261	- 3 0
ATOM	219	SG	CYS	25	23.700	18.417	51.184	1.000	17.82	
ANISOU	219	SG	CYS	25	1742	1825	3202	-122	-33	- 5 5
ATOM	220	N	LEU	26	24.623	16.308	48.250	1.000	15.25	
ANISOU	220	N	LEU	26	1449	1843	2504	-54	-263	- 1 4 2
ATOM	221	CA	LEU	26	23.560	15.590	47.534	1.000	15.62	
ANISOU	221	CA	LEU	26	1616	1739	2580	-86	-453	4 8
ATOM	222	C	LEU	26	23.763	14.085	47.621	1.000	15.18	
ANISOU	222	C	LEU	26	1697	1764	2306	-113	-479	6
ATOM	223	O	LEU	26	22.819	13.345	47.771	1.000	16.96	
ANISOU	223	O	LEU	26	1797	1725	2920	-234	-664	- 3 0 0
ATOM	224	CB	LEU	26	23.526	16.068	46.066	1.000	16.02	
ANISOU	224	CB	LEU	26	1811	1645	2633	-191	-483	1 2 2
ATOM	225	CG	LEU	26	23.057	17.510	45.864	1.000	15.69	
ANISOU	225	CG	LEU	26	1762	1716	2485	-6	-15	7 9
ATOM	226	CD1	LEU	26	23.252	17.880	44.405	1.000	17.48	
ANISOU	226	CD1	LEU	26	1750	2360	2532	-17	-130	4 6 5
ATOM	227	CD2	LEU	26	21.584	17.680	46.290	1.000	17.11	
ANISOU	227	CD2	LEU	26	1655	2188	2660	-29	-75	1 6 8
ATOM	228	N	ARG	27	25.027	13.648	47.494	1.000	17.26	
ANISOU	228	N	ARG	27	1870	1818	2871	155	-326	1 4 0
ATOM	229	CA	ARG	27	25.295	12.205	47.372	1.000	18.75	
ANISOU	229	CA	ARG	27	2108	1845	3170	270	-955	1 0 2
ATOM	230	C	ARG	27	25.240	11.599	48.744	1.000	17.95	
ANISOU	230	C	ARG	27	1667	1801	3351	159	-897	2 1 9
ATOM	231	O	ARG	27	24.777	10.454	48.913	1.000	20.99	
ANISOU	231	O	ARG	27	2158	1793	4026	-43	-360	1 6 8
ATOM	232	CB	ARG	27	26.641	12.008	46.670	1.000	21.35	
ANISOU	232	CB	ARG	27	2815	2034	3264	622	-377	- 1 2 9
ATOM	233	N	ASP	28	25.827	12.293	49.723	1.000	16.71	
ANISOU	233	N	ASP	28	1487	2004	2856	178	-328	6 7
ATOM	234	CA	ASP	28	26.034	11.672	51.026	1.000	17.47	
ANISOU	234	CA	ASP	28	1613	2095	2931	107	-301	1 2 7
ATOM	235	C	ASP	28	24.872	11.866	51.990	1.000	17.22	
ANISOU	235	C	ASP	28	1414	2264	2863	223	-447	4 7 1
ATOM	236	O	ASP	28	24.816	11.081	52.937	1.000	17.62	
ANISOU	236	O	ASP	28	1932	2139	2624	150	-565	3 2 7
ATOM	237	CB	ASP	28	27.306	12.237	51.657	1.000	22.17	
ANISOU	237	CB	ASP	28	1581	3894	2948	-272	-467	5 5 9
ATOM	238	CG	ASP	28	28.590	11.906	50.941	1.000	24.72	
ANISOU	238	CG	ASP	28	1596	3323	4472	236	-288	6 4 8
ATOM	239	OD1	ASP	28	28.572	10.905	50.199	1.000	27.56	
ANISOU	239	OD1	ASP	28	2317	3071	5084	808	-284	5 7 2
ATOM	240	OD2	ASP	28	29.573	12.617	51.251	1.000	32.08	
ANISOU	240	OD2	ASP	28	1584	4343	6261	-144	-470	4 1 6
ATOM	241	N	LYS	29	24.098	12.942	51.821	1.000	15.57	
ANISOU	241	N	LYS	29	1475	1814	2627	5	-303	1 7 8
ATOM	242	CA	LYS	29	23.048	13.305	52.778	1.000	15.13	
ANISOU	242	CA	LYS	29	1584	1999	2165	-68	-500	- 9 6
ATOM	243	C	LYS	29	21.686	13.500	52.118	1.000	14.56	
ANISOU	243	C	LYS	29	1496	1352	2686	77	-452	1 0 6
ATOM	244	O	LYS	29	20.688	12.985	52.635	1.000	16.21	
ANISOU	244	O	LYS	29	1627	1876	2657	-177	-315	- 5

- 21 -

ATOM	245	CB	LYS	29	23.431	14.563	53.574	1.000	16.09
ANISOU	245	CB	LYS	29	1666	1672	2777	3	-642 -25
ATOM	246	CG	LYS	29	24.776	14.421	54.292	1.000	17.68
ANISOU	246	CG	LYS	29	2192	1918	2606	7	-1144 141
ATOM	247	CD	LYS	29	25.161	15.647	55.096	1.000	20.71
ANISOU	247	CD	LYS	29	2675	2044	3151	-35	-1518 41
ATOM	248	CE	LYS	29	26.498	15.331	55.844	1.000	22.24
ANISOU	248	CE	LYS	29	2203	2714	3535	142	-1369 -685
ATOM	249	NZ	LYS	29	26.955	16.594	56.492	1.000	32.67
ANISOU	249	NZ	LYS	29	3199	3381	5831	-502	-2085 -1260
ATOM	250	N	GLY	30	21.604	14.198	50.993	1.000	14.09
ANISOU	250	N	GLY	30	1552	1461	2340	135	-455 -100
ATOM	251	CA	GLY	30	20.358	14.373	50.250	1.000	14.09
ANISOU	251	CA	GLY	30	1428	1561	2365	92	-342 -97
ATOM	252	C	GLY	30	19.372	15.284	50.955	1.000	12.30
ANISOU	252	C	GLY	30	1423	1192	2059	-95	-275 94
ATOM	253	O	GLY	30	18.168	15.223	50.696	1.000	14.58
ANISOU	253	O	GLY	30	1435	1689	2415	52	-476 -121
ATOM	254	N	LEU	31	19.884	16.146	51.823	1.000	13.93
ANISOU	254	N	LEU	31	1472	1479	2343	-182	-248 -181
ATOM	255	CA	LEU	31	19.012	17.114	52.511	1.000	14.44
ANISOU	255	CA	LEU	31	1534	1457	2495	-235	-55 -246
ATOM	256	C	LEU	31	19.894	18.286	52.942	1.000	15.08
ANISOU	256	C	LEU	31	1411	1535	2784	-177	-326 -314
ATOM	257	O	LEU	31	21.113	18.136	53.140	1.000	15.64
ANISOU	257	O	LEU	31	1468	1664	2812	-169	-328 -67
ATOM	258	CB	LEU	31	18.222	16.560	53.694	1.000	16.76
ANISOU	258	CB	LEU	31	2192	1664	2511	-367	128 -213
ATOM	259	CG	LEU	31	18.883	16.517	55.039	1.000	20.16
ANISOU	259	CG	LEU	31	2435	2485	2739	-289	-141 445
ATOM	260	CD1	LEU	31	17.977	16.145	56.202	1.000	26.49
ANISOU	260	CD1	LEU	31	2253	5076	2738	-508	-341 969
ATOM	261	CD2	LEU	31	20.052	15.526	55.032	1.000	24.73
ANISOU	261	CD2	LEU	31	4192	2967	2237	1001	153 610
ATOM	262	N	PHE	32	19.289	19.462	53.052	1.000	14.11
ANISOU	262	N	PHE	32	1569	1457	2335	-231	-179 -207
ATOM	263	CA	PHE	32	20.020	20.697	53.417	1.000	13.56
ANISOU	263	CA	PHE	32	1447	1389	2317	-225	-137 14
ATOM	264	C	PHE	32	18.976	21.777	53.687	1.000	13.72
ANISOU	264	C	PHE	32	1411	1439	2365	-218	-421 -142
ATOM	265	O	PHE	32	17.889	21.711	53.118	1.000	15.50
ANISOU	265	O	PHE	32	1392	1862	2634	-175	-436 -389
ATOM	266	CB	PHE	32	20.958	21.157	52.308	1.000	15.01
ANISOU	266	CB	PHE	32	1379	2201	2125	-305	-342 231
ATOM	267	CG	PHE	32	20.381	21.156	50.920	1.000	14.60
ANISOU	267	CG	PHE	32	1649	1662	2237	-193	-429 118
ATOM	268	CD1	PHE	32	20.326	19.986	50.148	1.000	14.53
ANISOU	268	CD1	PHE	32	1328	1688	2504	-156	-507 15
ATOM	269	CD2	PHE	32	19.831	22.345	50.396	1.000	13.66
ANISOU	269	CD2	PHE	32	1320	1678	2191	-179	-309 166
ATOM	270	CE1	PHE	32	19.742	20.033	48.892	1.000	14.26
ANISOU	270	CE1	PHE	32	1507	1655	2256	-346	-271 199
ATOM	271	CE2	PHE	32	19.267	22.348	49.138	1.000	15.49
ANISOU	271	CE2	PHE	32	1681	1932	2272	72	-504 -126
ATOM	272	CZ	PHE	32	19.177	21.184	48.385	1.000	15.25
ANISOU	272	CZ	PHE	32	1979	1700	2117	-185	-295 168
ATOM	273	N	TYR	33	19.376	22.785	54.442	1.000	14.44
ANISOU	273	N	TYR	33	1813	1302	2372	-237	-496 -50
ATOM	274	CA	TYR	33	18.616	24.023	54.519	1.000	14.32
ANISOU	274	CA	TYR	33	1764	1415	2261	-143	-295 -111
ATOM	275	C	TYR	33	19.039	24.929	53.364	1.000	13.70

- 22 -

ANISOU	275	C	TYR	33	1479	1565	2161	-79	-459	- 5
ATOM	276	O	TYR	33	20.158	24.871	52.859	1.000	15.28	
ANISOU	276	O	TYR	33	1370	1524	2912	-190	-420	2 6 3
ATOM	277	CB	TYR	33	18.874	24.734	55.853	1.000	14.47	
ANISOU	277	CB	TYR	33	1648	1717	2133	-197	-309	- 1 3 1
ATOM	278	CG	TYR	33	18.231	24.046	57.049	1.000	15.71	
ANISOU	278	CG	TYR	33	2131	1537	2302	-339	-109	- 1 3 6
ATOM	279	CD1	TYR	33	16.938	24.390	57.453	1.000	17.41	
ANISOU	279	CD1	TYR	33	2478	1967	2172	-154	246	- 2 4 9
ATOM	280	CD2	TYR	33	18.912	23.116	57.799	1.000	19.58	
ANISOU	280	CD2	TYR	33	2901	2070	2468	144	115	1 9 2
ATOM	281	CE1	TYR	33	16.354	23.758	58.542	1.000	20.18	
ANISOU	281	CE1	TYR	33	3138	1948	2581	26	740	- 1 0 2
ATOM	282	CE2	TYR	33	18.368	22.475	58.900	1.000	21.50	
ANISOU	282	CE2	TYR	33	3571	2480	2118	340	196	1 2 2
ATOM	283	CZ	TYR	33	17.081	22.821	59.263	1.000	22.02	
ANISOU	283	CZ	TYR	33	4140	1772	2454	471	1035	- 1 0 5
ATOM	284	OH	TYR	33	16.541	22.194	60.355	1.000	29.55	
ANISOU	284	OH	TYR	33	5088	2809	3329	377	1512	7 2 8
ATOM	285	N	LEU	34	18.076	25.709	52.878	1.000	14.28	
ANISOU	285	N	LEU	34	1496	1533	2396	-80	-517	- 1 7
ATOM	286	CA	LEU	34	18.278	26.620	51.756	1.000	15.02	
ANISOU	286	CA	LEU	34	1830	1452	2425	-126	-580	2 0
ATOM	287	C	LEU	34	17.871	28.039	52.151	1.000	14.46	
ANISOU	287	C	LEU	34	1703	1575	2217	-146	-241	- 7
ATOM	288	O	LEU	34	16.716	28.289	52.492	1.000	16.95	
ANISOU	288	O	LEU	34	1663	1852	2923	-75	-186	- 6 4
ATOM	289	CB	LEU	34	17.389	26.127	50.598	1.000	16.54	
ANISOU	289	CB	LEU	34	2355	1485	2444	-212	-749	2 5
ATOM	290	CG	LEU	34	17.633	26.800	49.249	1.000	15.65	
ANISOU	290	CG	LEU	34	2010	1567	2371	-7	-633	- 6 3
ATOM	291	CD1	LEU	34	18.977	26.422	48.664	1.000	20.14	
ANISOU	291	CD1	LEU	34	1919	2018	3717	-225	-171	2 6 0
ATOM	292	CD2	LEU	34	16.490	26.535	48.291	1.000	17.29	
ANISOU	292	CD2	LEU	34	2152	1824	2592	-425	-819	2 1 4
ATOM	293	N	THR	35	18.842	28.944	52.065	1.000	15.48	
ANISOU	293	N	THR	35	1817	1532	2534	-230	-200	1 3
ATOM	294	CA	THR	35	18.587	30.362	52.324	1.000	17.02	
ANISOU	294	CA	THR	35	2149	1537	2781	-206	-827	- 1 9 6
ATOM	295	C	THR	35	18.491	31.127	51.010	1.000	17.04	
ANISOU	295	C	THR	35	1895	1693	2887	-149	-882	- 4 4
ATOM	296	O	THR	35	18.765	30.572	49.938	1.000	17.01	
ANISOU	296	O	THR	35	1880	1692	2893	-262	-458	1 4 4
ATOM	297	CB	THR	35	19.772	30.917	53.180	1.000	17.79	
ANISOU	297	CB	THR	35	2018	1942	2800	-87	-854	- 2 0 0
ATOM	298	OG1	THR	35	20.986	30.673	52.474	1.000	21.10	
ANISOU	298	OG1	THR	35	2110	2035	3873	-253	-364	- 4 0 2
ATOM	299	CG2	THR	35	19.847	30.331	54.567	1.000	20.44	
ANISOU	299	CG2	THR	35	2600	2194	2971	228	-1113	5 9
ATOM	300	N	ASP	36	18.186	32.407	51.059	1.000	18.62	
ANISOU	300	N	ASP	36	2287	1747	3040	-187	-316	1 4 9
ATOM	301	CA	ASP	36	18.240	33.300	49.884	1.000	20.75	
ANISOU	301	CA	ASP	36	2678	1722	3483	-632	-508	3 7 4
ATOM	302	C	ASP	36	17.474	32.711	48.703	1.000	20.05	
ANISOU	302	C	ASP	36	2104	1929	3586	198	-928	4 8 9
ATOM	303	O	ASP	36	17.929	32.685	47.540	1.000	21.06	
ANISOU	303	O	ASP	36	2593	1749	3662	-496	-756	1 3 1
ATOM	304	CB	ASP	36	19.703	33.561	49.500	1.000	22.21	
ANISOU	304	CB	ASP	36	2666	2366	3406	-876	-755	8 0 7
ATOM	305	CG	ASP	36	20.588	34.192	50.551	1.000	23.05	
ANISOU	305	CG	ASP	36	2537	1818	4402	-175	-833	- 2 0 8

- 23 -

ATOM	306	OD1	ASP	36	20.061	34.886	51.457	1.000	26.16
ANISOU	306	OD1	ASP	36	2981	2100	4860	378	-777 -381
ATOM	307	OD2	ASP	36	21.824	33.982	50.528	1.000	24.87
ANISOU	307	OD2	ASP	36	2532	1994	4924	-49	-950 -628
ATOM	308	N	CYS	37	16.282	32.196	48.971	1.000	20.25
ANISOU	308	N	CYS	37	2135	1711	3849	118	-638 -263
ATOM	309	CA	CYS	37	15.463	31.587	47.902	1.000	20.28
ANISOU	309	CA	CYS	37	2390	1478	3839	136	-799 -138
ATOM	310	C	CYS	37	14.078	32.183	47.818	1.000	19.90
ANISOU	310	C	CYS	37	2374	1724	3463	214	-711 -74
ATOM	311	O	CYS	37	13.176	31.629	47.156	1.000	22.75
ANISOU	311	O	CYS	37	2569	1984	4091	-12	-1108 15
ATOM	312	CB	CYS	37	15.359	30.061	48.083	1.000	22.21
ANISOU	312	CB	CYS	37	2739	1454	4247	194	-477 -115
ATOM	313	SG	CYS	37	14.500	29.595	49.596	1.000	22.84
ANISOU	313	SG	CYS	37	2854	1884	3942	-203	-922 141
ATOM	314	N	GLY	38	13.855	33.390	48.314	1.000	20.85
ANISOU	314	N	GLY	38	2353	1638	3933	217	-375 -42
ATOM	315	CA	GLY	38	12.570	34.044	48.194	1.000	23.42
ANISOU	315	CA	GLY	38	2233	1874	4790	255	-292 165
ATOM	316	C	GLY	38	11.534	33.619	49.217	1.000	23.29
ANISOU	316	C	GLY	38	2577	2045	4228	113	-136 -601
ATOM	317	O	GLY	38	10.400	34.091	49.129	1.000	25.58
ANISOU	317	O	GLY	38	2529	3424	3765	214	-96 -264
ATOM	318	N	LEU	39	11.894	32.836	50.237	1.000	24.55
ANISOU	318	N	LEU	39	2310	2980	4037	119	-46 -364
ATOM	319	CA	LEU	39	10.938	32.331	51.195	1.000	24.44
ANISOU	319	CA	LEU	39	2637	2964	3684	-105	175 -946
ATOM	320	C	LEU	39	11.107	32.885	52.593	1.000	35.41
ANISOU	320	C	LEU	39	5341	4215	3898	-796	165 -1435
ATOM	321	O	LEU	39	11.784	32.313	53.441	1.000	43.41
ANISOU	321	O	LEU	39	7338	4986	4171	-2639	-1333 -303
ATOM	322	CB	LEU	39	10.850	30.810	51.206	1.000	26.48
ANISOU	322	CB	LEU	39	4244	2940	2879	49	-70 -261
ATOM	323	CG	LEU	39	10.404	30.097	49.921	1.000	30.21
ANISOU	323	CG	LEU	39	4834	2452	4195	258	-1618 -474
ATOM	324	CD1	LEU	39	10.683	28.595	49.972	1.000	24.78
ANISOU	324	CD1	LEU	39	3351	2597	3468	424	-707 -118
ATOM	325	CD2	LEU	39	8.940	30.407	49.640	1.000	27.50
ANISOU	325	CD2	LEU	39	4828	2118	3503	860	-860 -323
ATOM	326	N	THR	40	10.365	33.957	52.882	1.000	45.58
ANISOU	326	N	THR	40	7392	4849	5077	-520	2852 -1993
ATOM	327	CA	THR	40	10.610	34.661	54.136	1.000	32.50
ANISOU	327	CA	THR	40	4224	3732	4393	999	961 -558
ATOM	328	C	THR	40	9.700	34.177	55.248	1.000	29.68
ANISOU	328	C	THR	40	3175	4204	3898	-116	294 -1630
ATOM	329	O	THR	40	8.653	33.556	55.031	1.000	39.75
ANISOU	329	O	THR	40	3930	5847	5326	-1079	-301 -1653
ATOM	330	CB	THR	40	10.641	36.183	53.997	1.000	56.31
ANISOU	330	CB	THR	40	10586	3758	7052	-1417	1006 -992
ATOM	331	OG1	THR	40	11.545	36.606	52.946	1.000	68.39
ANISOU	331	OG1	THR	40	7379	3900	14707	-1978	3617 -246
ATOM	332	CG2	THR	40	11.214	36.837	55.256	1.000	70.22
ANISOU	332	CG2	THR	40	8265	5228	13188	1389	-4422 -3241
ATOM	333	N	ASP	41	10.191	34.302	56.486	1.000	33.20
ANISOU	333	N	ASP	41	3580	5223	3810	-203	307 -1779
ATOM	334	CA	ASP	41	9.329	33.943	57.613	1.000	27.51
ANISOU	334	CA	ASP	41	2705	3858	3891	91	-253 -1061
ATOM	335	C	ASP	41	8.107	34.861	57.660	1.000	33.43
ANISOU	335	C	ASP	41	3131	3064	6508	32	547 -1307
ATOM	336	O	ASP	41	7.034	34.469	58.101	1.000	30.76

- 24 -

ANISOU	336	O	ASP	41	2690	3223	5774	141	-149	-969
ATOM	337	CB	ASP	41	10.113	34.135	58.915	1.000	33.51	
ANISOU	337	CB	ASP	41	4853	4026	3852	-1222	-698	-938
ATOM	338	CG	ASP	41	9.453	33.351	60.039	1.000	33.37	
ANISOU	338	CG	ASP	41	3324	5291	4065	-739	-501	-571
ATOM	339	OD1	ASP	41	9.152	32.164	59.780	1.000	34.95	
ANISOU	339	OD1	ASP	41	4040	4681	4557	-380	824	-92
ATOM	340	OD2	ASP	41	9.395	33.904	61.161	1.000	86.76	
ANISOU	340	OD2	ASP	41	18972	10427	3567	-10425	588	-1858
ATOM	341	N	THR	42	8.272	36.089	57.205	1.000	32.71	
ANISOU	341	N	THR	42	3217	3695	5516	9	-58	-586
ATOM	342	CA	THR	42	7.198	37.074	57.221	1.000	38.48	
ANISOU	342	CA	THR	42	4747	4161	5711	1067	-861	-630
ATOM	343	C	THR	42	6.005	36.640	56.375	1.000	35.83	
ANISOU	343	C	THR	42	3333	4044	6237	1136	157	-1162
ATOM	344	O	THR	42	4.877	36.606	56.900	1.000	38.90	
ANISOU	344	O	THR	42	4048	3603	7128	1186	1059	1224
ATOM	345	CB	THR	42	7.751	38.449	56.815	1.000	37.05	
ANISOU	345	CB	THR	42	4526	3763	5788	1021	-677	-1532
ATOM	346	OG1	THR	42	8.831	38.301	55.889	1.000	98.08	
ANISOU	346	OG1	THR	42	16381	13757	7127	-3208	7500	-2318
ATOM	347	CG2	THR	42	8.358	39.113	58.047	1.000	36.08	
ANISOU	347	CG2	THR	42	6097	3613	3997	886	-1119	269
ATOM	348	N	GLU	43	6.259	36.184	55.173	1.000	34.64	
ANISOU	348	N	GLU	43	4208	3312	5642	656	-275	-698
ATOM	349	CA	GLU	43	5.391	35.557	54.192	1.000	32.98	
ANISOU	349	CA	GLU	43	3527	2886	6120	1199	-883	-152
ATOM	350	C	GLU	43	4.701	34.300	54.713	1.000	41.67	
ANISOU	350	C	GLU	43	3454	4151	8229	225	-1743	953
ATOM	351	O	GLU	43	3.484	34.124	54.605	1.000	38.53	
ANISOU	351	O	GLU	43	3375	4041	7222	589	-1417	-578
ATOM	352	CB	GLU	43	6.278	35.074	53.026	1.000	44.72	
ANISOU	352	CB	GLU	43	5991	4098	6901	28	137	-2137
ATOM	353	CG	GLU	43	6.658	36.125	52.003	1.000	53.42	
ANISOU	353	CG	GLU	43	5931	6417	7949	-993	1540	-1338
ATOM	354	CD	GLU	43	7.838	36.976	52.429	1.000	50.41	
ANISOU	354	CD	GLU	43	4087	7601	7467	-439	2486	-1725
ATOM	355	OE1	GLU	43	8.024	37.112	53.661	1.000	59.44	
ANISOU	355	OE1	GLU	43	7237	7592	7757	-1284	1632	-2146
ATOM	356	OE2	GLU	43	8.555	37.476	51.531	1.000	71.33	
ANISOU	356	OE2	GLU	43	11550	6344	9207	-4131	6267	-4645
ATOM	357	N	LEU	44	5.511	33.373	55.224	1.000	27.80	
ANISOU	357	N	LEU	44	2837	2924	4802	-55	-626	-227
ATOM	358	CA	LEU	44	4.926	32.222	55.902	1.000	27.88	
ANISOU	358	CA	LEU	44	2207	3379	5009	241	813	-382
ATOM	359	C	LEU	44	3.886	32.670	56.934	1.000	34.30	
ANISOU	359	C	LEU	44	1930	4771	6333	-537	776	-2629
ATOM	360	O	LEU	44	2.781	32.159	56.924	1.000	33.35	
ANISOU	360	O	LEU	44	2046	5235	5390	-840	705	-2397
ATOM	361	CB	LEU	44	5.999	31.394	56.587	1.000	24.59	
ANISOU	361	CB	LEU	44	2781	3494	3070	81	940	-74
ATOM	362	CG	LEU	44	5.592	30.147	57.343	1.000	31.76	
ANISOU	362	CG	LEU	44	2414	5135	4517	-845	792	1217
ATOM	363	CD1	LEU	44	4.563	29.328	56.575	1.000	47.71	
ANISOU	363	CD1	LEU	44	5860	7081	5188	-3576	3333	-2541
ATOM	364	CD2	LEU	44	6.793	29.259	57.653	1.000	51.56	
ANISOU	364	CD2	LEU	44	6294	3688	9608	1956	2240	1382
ATOM	365	N	LYS	45	4.212	33.712	57.694	1.000	41.91	
ANISOU	365	N	LYS	45	2865	6802	6256	-1455	381	-3537
ATOM	366	CA	LYS	45	3.369	34.195	58.773	1.000	44.31	
ANISOU	366	CA	LYS	45	4768	5427	6639	74	837	-2985

- 25 -

ATOM	367	C	LYS	45	1.981	34.582	58.278	1.000	38.58
ANISOU	367	C	LYS	45	4535	3445	6681	-245	1221 -2820
ATOM	368	O	LYS	45	0.984	34.238	58.902	1.000	39.93
ANISOU	368	O	LYS	45	4857	3594	6720	262	1634 -2337
ATOM	369	CB	LYS	45	4.038	35.400	59.447	1.000	50.20
ANISOU	369	CB	LYS	45	4944	5561	8569	1081	-447 -3980
ATOM	370	CG	LYS	45	3.082	36.546	59.706	1.000	53.07
ANISOU	370	CG	LYS	45	3548	6321	10296	1148	-2094 -4809
ATOM	371	CD	LYS	45	3.714	37.922	59.622	1.000	58.29
ANISOU	371	CD	LYS	45	4723	5694	11730	1422	-3745 -5024
ATOM	372	CE	LYS	45	3.199	38.793	60.761	1.000	65.33
ANISOU	372	CE	LYS	45	6294	6898	11629	1072	-3430 -5603
ATOM	373	NZ	LYS	45	1.713	38.779	60.852	1.000	73.75
ANISOU	373	NZ	LYS	45	6392	9216	12412	-718	-1071 -7436
ATOM	374	N	SER	46	1.973	35.341	57.193	1.000	36.94
ANISOU	374	N	SER	46	4074	3478	6484	-956	1068 -2939
ATOM	375	CA	SER	46	0.743	35.856	56.607	1.000	37.61
ANISOU	375	CA	SER	46	3983	3417	6892	-1335	988 -2335
ATOM	376	C	SER	46	-0.137	34.702	56.137	1.000	34.45
ANISOU	376	C	SER	46	3430	3057	6602	-1104	1656 -2394
ATOM	377	O	SER	46	-1.337	34.625	56.449	1.000	29.50
ANISOU	377	O	SER	46	3195	2789	5224	-587	1093 -1206
ATOM	378	CB	SER	46	1.160	36.726	55.419	1.000	40.36
ANISOU	378	CB	SER	46	4102	3809	7425	-2099	617 -1930
ATOM	379	OG	SER	46	0.018	37.017	54.630	1.000	43.38
ANISOU	379	OG	SER	46	5005	3431	8048	-1261	53 -1863
ATOM	380	N	ALA	47	0.493	33.808	55.361	1.000	29.82
ANISOU	380	N	ALA	47	3246	2173	5910	-18	809 -1228
ATOM	381	CA	ALA	47	-0.208	32.623	54.879	1.000	25.84
ANISOU	381	CA	ALA	47	3566	2106	4148	7 630	-891
ATOM	382	C	ALA	47	-0.722	31.792	56.058	1.000	25.02
ANISOU	382	C	ALA	47	2591	2344	4572	481	280 -280
ATOM	383	O	ALA	47	-1.888	31.381	56.063	1.000	23.19
ANISOU	383	O	ALA	47	2850	2366	3597	129	318 -1119
ATOM	384	CB	ALA	47	0.615	31.791	53.912	1.000	26.76
ANISOU	384	CB	ALA	47	2892	2764	4511	270	351 -1134
ATOM	385	N	LYS	48	0.132	31.529	57.041	1.000	24.64
ANISOU	385	N	LYS	48	3107	2076	4178	130	-57 -1085
ATOM	386	CA	LYS	48	-0.186	30.712	58.202	1.000	25.83
ANISOU	386	CA	LYS	48	3545	2979	3291	-16	30 -1416
ATOM	387	C	LYS	48	-1.337	31.339	59.003	1.000	28.58
ANISOU	387	C	LYS	48	3373	3344	4144	-354	129 -2041
ATOM	388	O	LYS	48	-2.310	30.694	59.396	1.000	27.04
ANISOU	388	O	LYS	48	3849	2793	3633	312	419 -634
ATOM	389	CB	LYS	48	1.035	30.654	59.149	1.000	28.95
ANISOU	389	CB	LYS	48	3507	3294	4200	-274	-257 -738
ATOM	390	CG	LYS	48	0.775	29.694	60.313	1.000	32.96
ANISOU	390	CG	LYS	48	4412	3214	4897	113	-543 -156
ATOM	391	CD	LYS	48	1.418	30.222	61.570	1.000	39.92
ANISOU	391	CD	LYS	48	5828	4616	4724	705	-1278 -39
ATOM	392	CE	LYS	48	1.217	29.320	62.769	1.000	33.67
ANISOU	392	CE	LYS	48	3973	4020	4799	1402	-205 -356
ATOM	393	NZ	LYS	48	0.731	30.100	63.946	1.000	38.33
ANISOU	393	NZ	LYS	48	4516	5230	4816	916	-1039 -1555
ATOM	394	N	ASP	49	-1.253	32.656	59.255	1.000	23.78
ANISOU	394	N	ASP	49	2796	3136	3104	79	-459 -1588
ATOM	395	CA	ASP	49	-2.298	33.326	60.006	1.000	24.05
ANISOU	395	CA	ASP	49	2826	2913	3398	-291	366 -1043
ATOM	396	C	ASP	49	-3.679	33.181	59.366	1.000	24.45
ANISOU	396	C	ASP	49	2721	3270	3300	-220	555 -1454
ATOM	397	O	ASP	49	-4.637	32.951	60.082	1.000	27.10

- 26 -

ANISOU	397	O	ASP	49	2863	3177	4257	-368	1004	-1544
ATOM	398	CB	ASP	49	-2.034	34.824	60.167	1.000	30.34	
ANISOU	398	CB	ASP	49	3695	3210	4623	-559	713	-2178
ATOM	399	CG	ASP	49	-0.924	35.181	61.128	1.000	37.18	
ANISOU	399	CG	ASP	49	5259	4057	4810	-1109	-211	-2007
ATOM	400	OD1	ASP	49	-0.556	34.266	61.904	1.000	33.36	
ANISOU	400	OD1	ASP	49	3717	4549	4408	-737	888	-1727
ATOM	401	OD2	ASP	49	-0.525	36.375	61.087	1.000	48.45	
ANISOU	401	OD2	ASP	49	7960	3575	6875	-927	-2887	-2409
ATOM	402	N	LEU	50	-3.788	33.402	58.059	1.000	24.46	
ANISOU	402	N	LEU	50	3114	2668	3513	374	200	-1298
ATOM	403	CA	LEU	50	-5.123	33.344	57.471	1.000	22.92	
ANISOU	403	CA	LEU	50	2949	2145	3614	161	397	-562
ATOM	404	C	LEU	50	-5.679	31.937	57.328	1.000	21.79	
ANISOU	404	C	LEU	50	3345	2197	2737	33	417	-556
ATOM	405	O	LEU	50	-6.878	31.741	57.475	1.000	24.96	
ANISOU	405	O	LEU	50	3463	2502	3517	-276	766	-1181
ATOM	406	CB	LEU	50	-5.254	34.137	56.194	1.000	22.13	
ANISOU	406	CB	LEU	50	3127	2016	3266	-103	524	-757
ATOM	407	CG	LEU	50	-6.661	34.578	55.807	1.000	28.87	
ANISOU	407	CG	LEU	50	3549	3538	3881	961	825	208
ATOM	408	CD1	LEU	50	-7.389	35.082	57.049	1.000	52.72	
ANISOU	408	CD1	LEU	50	4567	8556	6907	940	2929	-1936
ATOM	409	CD2	LEU	50	-6.644	35.642	54.723	1.000	41.07	
ANISOU	409	CD2	LEU	50	6971	3395	5240	-1005	-2258	857
ATOM	410	N	VAL	51	-4.801	30.956	57.138	1.000	21.78	
ANISOU	410	N	VAL	51	3345	2052	2877	-160	216	-860
ATOM	411	CA	VAL	51	-5.293	29.580	57.118	1.000	19.40	
ANISOU	411	CA	VAL	51	2631	2056	2683	-12	173	-303
ATOM	412	C	VAL	51	-5.631	29.135	58.533	1.000	25.25	
ANISOU	412	C	VAL	51	4453	2656	2485	-753	587	-955
ATOM	413	O	VAL	51	-6.652	28.454	58.725	1.000	25.07	
ANISOU	413	O	VAL	51	4555	2176	2795	-484	1185	-827
ATOM	414	CB	VAL	51	-4.377	28.589	56.396	1.000	18.78	
ANISOU	414	CB	VAL	51	2729	1786	2620	-72	171	-313
ATOM	415	CG1	VAL	51	-3.152	28.238	57.231	1.000	20.42	
ANISOU	415	CG1	VAL	51	3002	1841	2918	295	-13	-480
ATOM	416	CG2	VAL	51	-5.147	27.306	56.021	1.000	24.10	
ANISOU	416	CG2	VAL	51	3112	2337	3708	-511	355	-846
ATOM	417	N	ILE	52	-4.836	29.500	59.534	1.000	25.23	
ANISOU	417	N	ILE	52	4514	2471	2603	388	76	-874
ATOM	418	CA	ILE	52	-5.205	29.114	60.921	1.000	24.38	
ANISOU	418	CA	ILE	52	3488	3010	2765	248	19	-509
ATOM	419	C	ILE	52	-6.498	29.771	61.355	1.000	24.20	
ANISOU	419	C	ILE	52	3026	2482	3687	-354	114	-648
ATOM	420	O	ILE	52	-7.328	29.182	62.071	1.000	27.73	
ANISOU	420	O	ILE	52	3735	2812	3989	-198	614	-334
ATOM	421	CB	ILE	52	-4.016	29.427	61.829	1.000	27.59	
ANISOU	421	CB	ILE	52	3321	4347	2815	590	0	-785
ATOM	422	CG1	ILE	52	-2.853	28.439	61.510	1.000	31.45	
ANISOU	422	CG1	ILE	52	3278	5248	3425	741	363	-1288
ATOM	423	CG2	ILE	52	-4.293	29.312	63.317	1.000	33.62	
ANISOU	423	CG2	ILE	52	3827	6199	2750	881	150	-1454
ATOM	424	CD1	ILE	52	-1.930	28.351	62.710	1.000	36.22	
ANISOU	424	CD1	ILE	52	3956	5082	4722	979	-601	-234
ATOM	425	N	ASP	53	-6.771	30.992	60.913	1.000	24.56	
ANISOU	425	N	ASP	53	3479	2878	2974	165	609	-426
ATOM	426	CA	ASP	53	-8.051	31.646	61.278	1.000	23.50	
ANISOU	426	CA	ASP	53	3242	2942	2745	-5	355	-677
ATOM	427	C	ASP	53	-9.201	30.929	60.594	1.000	26.34	
ANISOU	427	C	ASP	53	3462	2986	3561	-435	612	-1064

- 27 -

ATOM	428	O	ASP	53	-10.342	30.836	61.051	1.000	29.73
ANISOU	428	O	ASP	53	3468	3085	4743	-436	937 -1142
ATOM	429	CB	ASP	53	-7.964	33.084	60.772	1.000	33.83
ANISOU	429	CB	ASP	53	3800	2322	6730	-92	1806 -933
ATOM	430	CG	ASP	53	-9.308	33.758	60.583	1.000	32.05
ANISOU	430	CG	ASP	53	4652	2412	5113	172	-302 -1138
ATOM	431	OD1	ASP	53	-9.653	34.524	61.486	1.000	43.68
ANISOU	431	OD1	ASP	53	3661	4686	8248	150	1379 -3120
ATOM	432	OD2	ASP	53	-9.950	33.556	59.532	1.000	51.30
ANISOU	432	OD2	ASP	53	8386	6074	5033	-2062	-1738 922
ATOM	433	N	PHE	54	-8.933	30.376	59.413	1.000	25.39
ANISOU	433	N	PHE	54	3372	2640	3637	72 71	-1176
ATOM	434	CA	PHE	54	-9.917	29.557	58.704	1.000	24.10
ANISOU	434	CA	PHE	54	3015	3264	2876	-366	263 -539
ATOM	435	C	PHE	54	-10.180	28.259	59.456	1.000	24.00
ANISOU	435	C	PHE	54	3264	3174	2680	-365	459 -688
ATOM	436	O	PHE	54	-11.333	27.893	59.686	1.000	28.19
ANISOU	436	O	PHE	54	3551	3246	3914	-549	1305 -1130
ATOM	437	CB	PHE	54	-9.465	29.273	57.263	1.000	23.62
ANISOU	437	CB	PHE	54	3241	2955	2779	-249	218 -434
ATOM	438	CG	PHE	54	-10.522	28.499	56.461	1.000	27.62
ANISOU	438	CG	PHE	54	4712	2945	2838	-694	-636 14
ATOM	439	CD1	PHE	54	-11.729	29.078	56.087	1.000	31.38
ANISOU	439	CD1	PHE	54	3613	4658	3654	-951	-262 -621
ATOM	440	CD2	PHE	54	-10.283	27.210	56.033	1.000	30.92
ANISOU	440	CD2	PHE	54	5782	3589	2377	-831	293 -844
ATOM	441	CE1	PHE	54	-12.653	28.406	55.307	1.000	44.29
ANISOU	441	CE1	PHE	54	5504	5404	5919	-3066	-2057 1178
ATOM	442	CE2	PHE	54	-11.228	26.503	55.306	1.000	38.69
ANISOU	442	CE2	PHE	54	7997	4412	2289	-2803	155 -387
ATOM	443	CZ	PHE	54	-12.424	27.092	54.927	1.000	42.33
ANISOU	443	CZ	PHE	54	5992	6305	3787	-4256	54 -446
ATOM	444	N	PHE	55	-9.126	27.558	59.870	1.000	25.87
ANISOU	444	N	PHE	55	3787	2768	3276	-85	431 -839
ATOM	445	CA	PHE	55	-9.195	26.310	60.625	1.000	25.69
ANISOU	445	CA	PHE	55	3567	3042	3151	68 763	-711
ATOM	446	C	PHE	55	-9.929	26.484	61.944	1.000	27.69
ANISOU	446	C	PHE	55	3357	3961	3205	181	703 -719
ATOM	447	O	PHE	55	-10.745	25.670	62.373	1.000	30.08
ANISOU	447	O	PHE	55	4046	4165	3217	142	878 -127
ATOM	448	CB	PHE	55	-7.759	25.873	60.932	1.000	25.48
ANISOU	448	CB	PHE	55	3556	3159	2964	117	835 -638
ATOM	449	CG	PHE	55	-7.019	25.242	59.762	1.000	26.31
ANISOU	449	CG	PHE	55	3437	3039	3522	-468	1068 -1156
ATOM	450	CD1	PHE	55	-7.611	24.820	58.590	1.000	27.09
ANISOU	450	CD1	PHE	55	3553	3895	2845	-1018	1404 -658
ATOM	451	CD2	PHE	55	-5.651	25.031	59.935	1.000	31.68
ANISOU	451	CD2	PHE	55	3244	4185	4609	-726	1123 -2221
ATOM	452	CE1	PHE	55	-6.878	24.150	57.621	1.000	23.89
ANISOU	452	CE1	PHE	55	3472	2525	3079	-58	551 -547
ATOM	453	CE2	PHE	55	-4.904	24.433	58.950	1.000	31.74
ANISOU	453	CE2	PHE	55	3487	4387	4186	226	337 -2304
ATOM	454	CZ	PHE	55	-5.514	24.004	57.770	1.000	24.23
ANISOU	454	CZ	PHE	55	3706	2187	3312	414	-22 -416
ATOM	455	N	GLU	56	-9.633	27.581	62.629	1.000	30.39
ANISOU	455	N	GLU	56	3961	5033	2553	-308	520 -1110
ATOM	456	CA	GLU	56	-10.222	27.875	63.925	1.000	30.18
ANISOU	456	CA	GLU	56	4160	4504	2805	-734	1221 -637
ATOM	457	C	GLU	56	-11.650	28.401	63.820	1.000	33.50
ANISOU	457	C	GLU	56	4324	4124	4280	-535	1489 -892
ATOM	458	O	GLU	56	-12.470	28.149	64.708	1.000	44.44

- 28 -

ANISOU	458	O	GLU	56	3864	8872	4150	93	1013	1011
ATOM	459	CB	GLU	56	-9.403	28.978	64.615	1.000	35.85	
ANISOU	459	CB	GLU	56	5037	5109	3475	-221	574	-1821
ATOM	460	CG	GLU	56	-8.192	28.508	65.401	1.000	38.63	
ANISOU	460	CG	GLU	56	4804	7152	2721	-337	763	-1692
ATOM	461	CD	GLU	56	-7.395	29.699	65.916	1.000	45.55	
ANISOU	461	CD	GLU	56	5576	7183	4546	-24	-295	-2330
ATOM	462	OE1	GLU	56	-7.935	30.828	65.888	1.000	55.54	
ANISOU	462	OE1	GLU	56	7344	7247	6512	586	2570	-3059
ATOM	463	OE2	GLU	56	-6.246	29.492	66.350	1.000	50.41	
ANISOU	463	OE2	GLU	56	4050	10497	4606	-1066	1163	-2063
ATOM	464	N	HIS	57	-11.890	29.289	62.866	1.000	32.20	
ANISOU	464	N	HIS	57	3273	4700	4261	-549	1540	-670
ATOM	465	CA	HIS	57	-13.101	30.078	62.909	1.000	33.38	
ANISOU	465	CA	HIS	57	3795	4885	4002	-110	1553	-1239
ATOM	466	C	HIS	57	-13.981	29.873	61.697	1.000	32.85	
ANISOU	466	C	HIS	57	3380	4736	4367	278	1506	-1797
ATOM	467	O	HIS	57	-15.012	30.533	61.571	1.000	37.09	
ANISOU	467	O	HIS	57	3362	4733	5998	276	1087	-2205
ATOM	468	CB	HIS	57	-12.802	31.573	62.976	1.000	37.39	
ANISOU	468	CB	HIS	57	4327	4959	4922	-193	1402	-1970
ATOM	469	CG	HIS	57	-11.981	31.949	64.162	1.000	36.99	
ANISOU	469	CG	HIS	57	4111	5046	4896	680	1344	-2319
ATOM	470	ND1	HIS	57	-12.465	31.917	65.453	1.000	38.84	
ANISOU	470	ND1	HIS	57	5090	4844	4823	-171	1362	-1598
ATOM	471	CD2	HIS	57	-10.707	32.387	64.232	1.000	37.91	
ANISOU	471	CD2	HIS	57	5259	4197	4947	-891	1544	-2828
ATOM	472	CE1	HIS	57	-11.510	32.305	66.275	1.000	40.37	
ANISOU	472	CE1	HIS	57	5481	5191	4668	-243	1087	-1361
ATOM	473	NE2	HIS	57	-10.441	32.592	65.552	1.000	35.63	
ANISOU	473	NE2	HIS	57	4420	4376	4743	980	799	-1492
ATOM	474	N	GLY	58	-13.464	29.068	60.786	1.000	32.06	
ANISOU	474	N	GLY	58	4402	3186	4594	5	1572	-1525
ATOM	475	CA	GLY	58	-14.290	28.731	59.627	1.000	35.74	
ANISOU	475	CA	GLY	58	4508	4402	4669	-1129	1877	-1893
ATOM	476	C	GLY	58	-15.449	27.859	60.099	1.000	31.52	
ANISOU	476	C	GLY	58	3317	3688	4969	308	1657	-593
ATOM	477	O	GLY	58	-15.245	26.952	60.922	1.000	32.66	
ANISOU	477	O	GLY	58	4561	4176	3674	-204	624	-1012
ATOM	478	N	SER	59	-16.632	28.152	59.574	1.000	31.03	
ANISOU	478	N	SER	59	3786	3623	4379	519	1142	-1442
ATOM	479	CA	SER	59	-17.823	27.359	59.859	1.000	32.03	
ANISOU	479	CA	SER	59	3305	3925	4939	757	850	-1188
ATOM	480	C	SER	59	-17.763	26.034	59.117	1.000	37.27	
ANISOU	480	C	SER	59	3654	4001	6507	0	2065	-1682
ATOM	481	O	SER	59	-16.987	25.858	58.181	1.000	31.23	
ANISOU	481	O	SER	59	3027	3655	5184	613	1003	-1174
ATOM	482	CB	SER	59	-19.077	28.136	59.444	1.000	39.80	
ANISOU	482	CB	SER	59	3930	5925	5266	1707	-545	-2846
ATOM	483	OG	SER	59	-19.252	28.159	58.029	1.000	35.38	
ANISOU	483	OG	SER	59	3505	4800	5137	355	119	-1624
ATOM	484	N	GLU	60	-18.589	25.065	59.507	1.000	46.32	
ANISOU	484	N	GLU	60	5438	6083	6078	-2395	2115	-2700
ATOM	485	CA	GLU	60	-18.573	23.801	58.754	1.000	34.21	
ANISOU	485	CA	GLU	60	3381	4798	4818	-960	716	-1238
ATOM	486	C	GLU	60	-19.033	24.055	57.330	1.000	34.22	
ANISOU	486	C	GLU	60	4659	3711	4632	455	1378	-847
ATOM	487	O	GLU	60	-18.616	23.437	56.361	1.000	29.91	
ANISOU	487	O	GLU	60	3708	3040	4615	-679	2037	-604
ATOM	488	CB	GLU	60	-19.390	22.742	59.488	1.000	38.26	
ANISOU	488	CB	GLU	60	5012	5567	3958	-1599	748	-1000

- 29 -

ATOM	489	CG	GLU	60	-18.625	22.182	60.678	1.000	42.01
ANISOU	489	CG	GLU	60	5470	5439	5055	503	950 - 7 8 2
ATOM	490	CD	GLU	60	-17.307	21.528	60.312	1.000	45.34
ANISOU	490	CD	GLU	60	4036	7496	5695	-885	1094 - 2 2 7 6
ATOM	491	OE1	GLU	60	-17.219	20.867	59.264	1.000	49.69
ANISOU	491	OE1	GLU	60	5383	6689	6809	-864	1730 - 2 8 3 8
ATOM	492	OE2	GLU	60	-16.323	21.659	61.084	1.000	43.62
ANISOU	492	OE2	GLU	60	4677	4974	6924	-1984	109 - 1 2
ATOM	493	N	ALA	61	-19.928	25.028	57.167	1.000	34.26
ANISOU	493	N	ALA	61	3091	3912	6014	-81	1209 - 1 1 2 2
ATOM	494	CA	ALA	61	-20.408	25.324	55.823	1.000	33.07
ANISOU	494	CA	ALA	61	1647	4409	6508	-228	657 - 1 1 0 5
ATOM	495	C	ALA	61	-19.314	25.876	54.938	1.000	30.69
ANISOU	495	C	ALA	61	2053	3742	5866	-59	640 - 1 0 6 6
ATOM	496	O	ALA	61	-19.138	25.482	53.790	1.000	31.15
ANISOU	496	O	ALA	61	2754	2893	6189	31 793	- 1 2 8 5
ATOM	497	CB	ALA	61	-21.543	26.336	55.932	1.000	34.43
ANISOU	497	CB	ALA	61	2783	4403	5897	288	1210 - 1 6 5 0
ATOM	498	N	GLU	62	-18.568	26.824	55.498	1.000	28.80
ANISOU	498	N	GLU	62	2168	3404	5371	-9 915	- 9 6 4
ATOM	499	CA	GLU	62	-17.478	27.395	54.704	1.000	26.78
ANISOU	499	CA	GLU	62	2339	2374	5461	423	871 - 4 1 3
ATOM	500	C	GLU	62	-16.432	26.330	54.389	1.000	22.61
ANISOU	500	C	GLU	62	2569	1621	4402	84 1049	- 3 7 6
ATOM	501	O	GLU	62	-15.851	26.316	53.289	1.000	24.41
ANISOU	501	O	GLU	62	2399	2669	4209	-132	801 - 5 4 8
ATOM	502	CB	GLU	62	-16.861	28.591	55.429	1.000	32.86
ANISOU	502	CB	GLU	62	3129	2117	7239	251	2039 - 1 3 5 8
ATOM	503	CG	GLU	62	-17.739	29.834	55.554	1.000	34.69
ANISOU	503	CG	GLU	62	2824	2859	7499	916	-95 - 1 4 3 0
ATOM	504	CD	GLU	62	-17.274	30.810	56.616	1.000	38.93
ANISOU	504	CD	GLU	62	4998	2780	7014	1622	224 - 1 8 2 0
ATOM	505	OE1	GLU	62	-16.861	30.391	57.717	1.000	40.92
ANISOU	505	OE1	GLU	62	4844	3636	7068	1268	34 - 1 6 7 3
ATOM	506	OE2	GLU	62	-17.324	32.041	56.385	1.000	45.13
ANISOU	506	OE2	GLU	62	7600	2889	6658	-525	1698 - 1 0 9 9
ATOM	507	N	LYS	63	-16.193	25.431	55.345	1.000	25.20
ANISOU	507	N	LYS	63	2470	2380	4723	312	1050 8
ATOM	508	CA	LYS	63	-15.214	24.369	55.207	1.000	21.62
ANISOU	508	CA	LYS	63	2608	2894	2712	688	349 - 4 4 6
ATOM	509	C	LYS	63	-15.708	23.397	54.147	1.000	22.42
ANISOU	509	C	LYS	63	2930	3038	2549	84 433	- 2 1 7
ATOM	510	O	LYS	63	-14.913	23.038	53.289	1.000	24.17
ANISOU	510	O	LYS	63	3340	2354	3491	239	782 - 7 9 0
ATOM	511	CB	LYS	63	-14.940	23.650	56.534	1.000	24.50
ANISOU	511	CB	LYS	63	3411	3057	2842	42 - 105	- 2 9 9
ATOM	512	CG	LYS	63	-13.963	24.465	57.381	1.000	27.58
ANISOU	512	CG	LYS	63	4640	2792	3045	-302	-465 - 3 0 6
ATOM	513	CD	LYS	63	-13.866	23.937	58.811	1.000	26.09
ANISOU	513	CD	LYS	63	3132	3570	3211	305	-575 - 1 2
ATOM	514	CE	LYS	63	-12.761	24.695	59.560	1.000	28.96
ANISOU	514	CE	LYS	63	4342	3579	3083	-317	-286 - 7 9 2
ATOM	515	NZ	LYS	63	-12.927	24.614	61.030	1.000	35.00
ANISOU	515	NZ	LYS	63	4884	5356	3057	64 - 298	- 8 1 7
ATOM	516	N	ARG	64	-17.007	23.112	54.143	1.000	29.82
ANISOU	516	N	ARG	64	3238	2676	5418	-533	1111 - 1 2 5 9
ATOM	517	CA	ARG	64	-17.521	22.169	53.118	1.000	25.56
ANISOU	517	CA	ARG	64	2396	2474	4841	-170	1252 - 9 6 2
ATOM	518	C	ARG	64	-17.417	22.735	51.708	1.000	28.45
ANISOU	518	C	ARG	64	3022	2681	5106	153	1369 - 5 6 2
ATOM	519	O	ARG	64	-17.149	21.981	50.759	1.000	22.57

- 30 -

ANISOU	519	O	ARG	64	1672	2466	4436	-71	148	-395
ATOM	520	CB	ARG	64	-18.937	21.809	53.537	1.000	32.48	
ANISOU	520	CB	ARG	64	2669	4144	5526	-809	1483	-1029
ATOM	521	CG	ARG	64	-19.094	20.442	54.189	1.000	45.55	
ANISOU	521	CG	ARG	64	4444	4749	8116	-2443	1343	-153
ATOM	522	CD	ARG	64	-20.557	19.985	54.080	1.000	59.48	
ANISOU	522	CD	ARG	64	5723	6760	10116	-3977	-2863	2461
ATOM	523	NE	ARG	64	-20.759	19.485	52.714	1.000	77.63	
ANISOU	523	NE	ARG	64	10254	9303	9938	-4031	-4193	2666
ATOM	524	CZ	ARG	64	-21.166	20.236	51.696	1.000	60.23	
ANISOU	524	CZ	ARG	64	5289	6952	10644	-1128	-4334	501
ATOM	525	NH1	ARG	64	-21.424	21.528	51.892	1.000	91.64	
ANISOU	525	NH1	ARG	64	18286	5072	11461	-5082	-3134	-75
ATOM	526	NH2	ARG	64	-21.286	19.711	50.489	1.000	43.67	
ANISOU	526	NH2	ARG	64	3318	4095	9178	-183	-1521	2085
ATOM	527	N	ALA	65	-17.624	24.041	51.515	1.000	26.71	
ANISOU	527	N	ALA	65	1907	2770	5472	189	936	-556
ATOM	528	CA	ALA	65	-17.522	24.661	50.199	1.000	24.91	
ANISOU	528	CA	ALA	65	1798	2379	5288	280	417	-754
ATOM	529	C	ALA	65	-16.109	24.575	49.595	1.000	21.81	
ANISOU	529	C	ALA	65	1808	2408	4071	597	155	-626
ATOM	530	O	ALA	65	-15.935	24.724	48.381	1.000	24.13	
ANISOU	530	O	ALA	65	2127	3076	3964	224	-220	-485
ATOM	531	CB	ALA	65	-18.023	26.096	50.221	1.000	31.78	
ANISOU	531	CB	ALA	65	3096	2984	5993	1337	1401	-453
ATOM	532	N	VAL	66	-15.098	24.306	50.426	1.000	19.29	
ANISOU	532	N	VAL	66	1836	1880	3614	466	360	-541
ATOM	533	CA	VAL	66	-13.723	24.167	49.953	1.000	18.17	
ANISOU	533	CA	VAL	66	1636	1653	3616	204	79	-487
ATOM	534	C	VAL	66	-13.166	22.767	50.248	1.000	15.18	
ANISOU	534	C	VAL	66	1516	1638	2613	120	126	-571
ATOM	535	O	VAL	66	-11.959	22.623	50.353	1.000	17.63	
ANISOU	535	O	VAL	66	1567	2071	3060	217	-106	-317
ATOM	536	CB	VAL	66	-12.784	25.277	50.437	1.000	18.91	
ANISOU	536	CB	VAL	66	2175	1576	3433	183	-135	-598
ATOM	537	CG1	VAL	66	-13.139	26.627	49.805	1.000	20.60	
ANISOU	537	CG1	VAL	66	2067	1751	4010	219	593	-83
ATOM	538	CG2	VAL	66	-12.736	25.373	51.945	1.000	21.61	
ANISOU	538	CG2	VAL	66	2689	2066	3455	102	22	-603
ATOM	539	N	THR	67	-14.048	21.792	50.343	1.000	18.30	
ANISOU	539	N	THR	67	1761	1614	3577	-20	-6	-514
ATOM	540	CA	THR	67	-13.673	20.403	50.563	1.000	17.18	
ANISOU	540	CA	THR	67	1927	1656	2946	-32	50	-556
ATOM	541	C	THR	67	-13.979	19.566	49.332	1.000	16.52	
ANISOU	541	C	THR	67	1763	1742	2773	21	27	-467
ATOM	542	O	THR	67	-15.107	19.613	48.811	1.000	18.13	
ANISOU	542	O	THR	67	1750	2211	2929	73	-86	-383
ATOM	543	CB	THR	67	-14.373	19.791	51.782	1.000	18.54	
ANISOU	543	CB	THR	67	2202	2014	2827	192	224	-492
ATOM	544	OG1	THR	67	-14.060	20.554	52.961	1.000	20.14	
ANISOU	544	OG1	THR	67	2481	2251	2920	-108	155	-468
ATOM	545	CG2	THR	67	-13.912	18.364	52.017	1.000	20.04	
ANISOU	545	CG2	THR	67	2393	2016	3203	29	-86	-235
ATOM	546	N	SER	68	-13.030	18.818	48.821	1.000	16.71	
ANISOU	546	N	SER	68	1612	1720	3018	-135	154	-498
ATOM	547	CA	SER	68	-13.281	17.947	47.688	1.000	16.33	
ANISOU	547	CA	SER	68	1508	1631	3065	-184	365	-561
ATOM	548	C	SER	68	-14.223	16.795	48.057	1.000	14.85	
ANISOU	548	C	SER	68	1194	1775	2672	-81	197	-448
ATOM	549	O	SER	68	-14.303	16.431	49.233	1.000	16.36	
ANISOU	549	O	SER	68	1783	1775	2659	-145	192	-481

- 31 -

ATOM	550	CB	SER	68	-11.958	17.303	47.257	1.000	17.84
ANISOU	550	CB	SER	68	1459	2139	3182	-87	647 -313
ATOM	551	OG	SER	68	-10.998	18.259	46.904	1.000	17.21
ANISOU	551	OG	SER	68	1659	1987	2893	-75	364 -49
ATOM	552	N	PRO	69	-14.929	16.284	47.054	1.000	15.89
ANISOU	552	N	PRO	69	1574	1661	2803	-201	-103 -280
ATOM	553	CA	PRO	69	-15.877	15.182	47.339	1.000	16.42
ANISOU	553	CA	PRO	69	1428	1903	2908	-251	-148 -218
ATOM	554	C	PRO	69	-15.168	13.889	47.684	1.000	17.22
ANISOU	554	C	PRO	69	1633	1578	3331	-199	266 -424
ATOM	555	O	PRO	69	-15.794	12.997	48.287	1.000	18.35
ANISOU	555	O	PRO	69	1815	1760	3399	-365	232 -376
ATOM	556	CB	PRO	69	-16.712	15.057	46.060	1.000	16.75
ANISOU	556	CB	PRO	69	1354	2279	2733	-360	155 -729
ATOM	557	CG	PRO	69	-15.799	15.637	45.008	1.000	16.72
ANISOU	557	CG	PRO	69	1553	1971	2827	-359	38 -452
ATOM	558	CD	PRO	69	-15.059	16.797	45.681	1.000	17.10
ANISOU	558	CD	PRO	69	1918	1804	2776	-344	-119 -313
ATOM	559	N	VAL	70	-13.884	13.746	47.366	1.000	18.07
ANISOU	559	N	VAL	70	1716	1764	3384	-89	292 -215
ATOM	560	CA	VAL	70	-13.100	12.594	47.824	1.000	17.34
ANISOU	560	CA	VAL	70	1763	1851	2974	-20	260 -196
ATOM	561	C	VAL	70	-11.995	13.142	48.720	1.000	17.59
ANISOU	561	C	VAL	70	2207	1686	2788	-180	159 -142
ATOM	562	O	VAL	70	-11.431	14.186	48.389	1.000	18.59
ANISOU	562	O	VAL	70	1794	1688	3581	-49	152
ATOM	563	CB	VAL	70	-12.429	11.757	46.724	1.000	18.10
ANISOU	563	CB	VAL	70	1922	1756	3199	-353	560 -446
ATOM	564	CG1	VAL	70	-13.441	10.754	46.213	1.000	20.54
ANISOU	564	CG1	VAL	70	1927	2611	3268	-369	76 -663
ATOM	565	CG2	VAL	70	-11.760	12.608	45.642	1.000	17.65
ANISOU	565	CG2	VAL	70	2379	1806	2520	145	9 10
ATOM	566	N	PRO	71	-11.697	12.466	49.815	1.000	16.21
ANISOU	566	N	PRO	71	1653	1810	2695	-34	464 -156
ATOM	567	CA	PRO	71	-10.839	13.091	50.833	1.000	17.32
ANISOU	567	CA	PRO	71	1795	1931	2854	-121	184 -12
ATOM	568	C	PRO	71	-9.356	12.804	50.590	1.000	17.67
ANISOU	568	C	PRO	71	1865	1927	2921	46	-57 156
ATOM	569	O	PRO	71	-8.585	12.223	51.350	1.000	20.57
ANISOU	569	O	PRO	71	2218	2247	3350	424	28 474
ATOM	570	CB	PRO	71	-11.362	12.458	52.117	1.000	19.76
ANISOU	570	CB	PRO	71	2976	1862	2668	-347	479 -304
ATOM	571	CG	PRO	71	-11.721	11.056	51.670	1.000	19.08
ANISOU	571	CG	PRO	71	2838	1805	2608	-267	259 -234
ATOM	572	CD	PRO	71	-12.323	11.220	50.286	1.000	17.97
ANISOU	572	CD	PRO	71	2314	1974	2538	-390	451 -167
ATOM	573	N	THR	72	-8.894	13.338	49.446	1.000	17.15
ANISOU	573	N	THR	72	1677	2231	2610	-215	-17 -165
ATOM	574	CA	THR	72	-7.573	13.012	48.935	1.000	16.83
ANISOU	574	CA	THR	72	1721	1863	2810	-60	-134 -472
ATOM	575	C	THR	72	-6.490	14.000	49.358	1.000	15.20
ANISOU	575	C	THR	72	1791	1623	2362	-304	163 -73
ATOM	576	O	THR	72	-5.320	13.729	49.104	1.000	17.49
ANISOU	576	O	THR	72	1776	1961	2908	-61	-31 -225
ATOM	577	CB	THR	72	-7.533	12.971	47.399	1.000	16.18
ANISOU	577	CB	THR	72	1552	1848	2748	-146	-86 -261
ATOM	578	OG1	THR	72	-8.091	14.238	47.005	1.000	17.81
ANISOU	578	OG1	THR	72	1856	1880	3031	-34	115 -191
ATOM	579	CG2	THR	72	-8.338	11.816	46.825	1.000	17.49
ANISOU	579	CG2	THR	72	1953	2087	2605	-550	181 -329
ATOM	580	N	MET	73	-6.877	15.098	49.987	1.000	17.78

ANISOU	580	N	MET	73	2057	1748	2951	-58	-254	-426
ATOM	581	CA	MET	73	-5.867	16.117	50.394	1.000	16.58	
ANISOU	581	CA	MET	73	1796	1708	2797	88	-302	-340
ATOM	582	C	MET	73	-5.073	16.618	49.198	1.000	16.65	
ANISOU	582	C	MET	73	1514	1787	3027	241	-162	-420
ATOM	583	O	MET	73	-3.911	17.039	49.292	1.000	19.39	
ANISOU	583	O	MET	73	1705	2313	3348	-112	-240	-540
ATOM	584	CB	MET	73	-4.925	15.531	51.469	1.000	20.56	
ANISOU	584	CB	MET	73	2099	2629	3083	345	-507	-286
ATOM	585	CG	MET	73	-5.703	15.154	52.715	1.000	30.33	
ANISOU	585	CG	MET	73	3008	5133	3384	-69	-609	1027
ATOM	586	SD	MET	73	-4.692	14.263	53.891	1.000	36.13	
ANISOU	586	SD	MET	73	4121	5050	4558	336	-918	1596
ATOM	587	CE	MET	73	-3.165	13.987	53.082	1.000	58.07	
ANISOU	587	CE	MET	73	2810	8820	10435	975	-1592	-3138
ATOM	588	N	ARG	74	-5.687	16.632	48.025	1.000	16.83	
ANISOU	588	N	ARG	74	1699	1714	2982	-6	-211	131
ATOM	589	CA	ARG	74	-5.099	17.215	46.817	1.000	15.87	
ANISOU	589	CA	ARG	74	1365	1618	3046	-17	52	-325
ATOM	590	C	ARG	74	-5.359	18.714	46.761	1.000	14.22	
ANISOU	590	C	ARG	74	1484	1651	2269	141	-32	-42
ATOM	591	O	ARG	74	-4.472	19.488	46.353	1.000	15.45	
ANISOU	591	O	ARG	74	1525	1758	2586	-12	-46	-73
ATOM	592	CB	ARG	74	-5.675	16.530	45.566	1.000	15.68	
ANISOU	592	CB	ARG	74	1330	1667	2959	160	-14	-311
ATOM	593	CG	ARG	74	-4.890	16.941	44.299	1.000	16.46	
ANISOU	593	CG	ARG	74	1325	1870	3059	-175	55	-395
ATOM	594	CD	ARG	74	-5.655	16.396	43.072	1.000	16.37	
ANISOU	594	CD	ARG	74	1789	1533	2899	-181	-8	-177
ATOM	595	NE	ARG	74	-4.840	16.601	41.857	1.000	19.21	
ANISOU	595	NE	ARG	74	2289	1990	3020	-142	241	-156
ATOM	596	CZ	ARG	74	-4.944	17.626	41.039	1.000	17.00	
ANISOU	596	CZ	ARG	74	1545	2351	2562	-67	26	-147
ATOM	597	NH1	ARG	74	-5.878	18.573	41.213	1.000	18.00	
ANISOU	597	NH1	ARG	74	1818	2383	2638	51	-66	-220
ATOM	598	NH2	ARG	74	-4.144	17.703	39.987	1.000	20.50	
ANISOU	598	NH2	ARG	74	2285	2972	2532	-110	310	-387
ATOM	599	N	ARG	75	-6.579	19.151	47.101	1.000	15.28	
ANISOU	599	N	ARG	75	1755	1544	2507	137	340	-173
ATOM	600	CA	ARG	75	-6.999	20.550	46.980	1.000	14.68	
ANISOU	600	CA	ARG	75	1679	1627	2272	236	98	-150
ATOM	601	C	ARG	75	-7.956	20.869	48.122	1.000	14.75	
ANISOU	601	C	ARG	75	1445	1747	2414	124	133	-233
ATOM	602	O	ARG	75	-8.760	19.989	48.460	1.000	18.12	
ANISOU	602	O	ARG	75	1677	2109	3101	-156	458	-433
ATOM	603	CB	ARG	75	-7.747	20.804	45.668	1.000	15.59	
ANISOU	603	CB	ARG	75	1577	2030	2317	1	46	-106
ATOM	604	CG	ARG	75	-6.848	20.634	44.441	1.000	15.63	
ANISOU	604	CG	ARG	75	1495	2110	2334	9	147	220
ATOM	605	CD	ARG	75	-5.712	21.618	44.334	1.000	15.59	
ANISOU	605	CD	ARG	75	1658	1792	2475	11	130	-10
ATOM	606	NE	ARG	75	-5.061	21.601	43.011	1.000	15.25	
ANISOU	606	NE	ARG	75	1421	1779	2596	122	227	144
ATOM	607	CZ	ARG	75	-3.957	20.865	42.732	1.000	14.90	
ANISOU	607	CZ	ARG	75	1079	2361	2221	71	-86	242
ATOM	608	NH1	ARG	75	-3.405	20.091	43.664	1.000	16.18	
ANISOU	608	NH1	ARG	75	1804	1722	2623	-134	-387	337
ATOM	609	NH2	ARG	75	-3.418	20.940	41.518	1.000	15.83	
ANISOU	609	NH2	ARG	75	1677	2107	2232	-193	221	0
ATOM	610	N	GLY	76	-7.895	22.086	48.651	1.000	16.06	
ANISOU	610	N	GLY	76	1686	1904	2513	109	220	-464

- 33 -

ATOM	611	CA	GLY	76	-8.858	22.532	49.637	1.000	16.67	
ANISOU	611	CA	GLY	76	1650	2260	2425	-70	199	-612
ATOM	612	C	GLY	76	-8.602	22.002	51.036	1.000	16.32	
ANISOU	612	C	GLY	76	1584	2014	2602	-126	268	-347
ATOM	613	O	GLY	76	-7.469	21.651	51.370	1.000	16.87	
ANISOU	613	O	GLY	76	1638	1998	2773	-45	308	-218
ATOM	614	N	PHE	77	-9.643	22.025	51.863	1.000	16.88	
ANISOU	614	N	PHE	77	1597	2141	2675	-7	283	-191
ATOM	615	CA	PHE	77	-9.584	21.646	53.274	1.000	17.61	
ANISOU	615	CA	PHE	77	1838	2196	2656	109	328	-114
ATOM	616	C	PHE	77	-9.776	20.154	53.512	1.000	17.64	
ANISOU	616	C	PHE	77	1855	2248	2600	-68	243	-185
ATOM	617	O	PHE	77	-10.589	19.528	52.831	1.000	18.23	
ANISOU	617	O	PHE	77	1844	2488	2594	-183	357	-240
ATOM	618	CB	PHE	77	-10.698	22.383	53.998	1.000	17.70	
ANISOU	618	CB	PHE	77	1730	2515	2480	162	65	-344
ATOM	619	CG	PHE	77	-10.877	22.081	55.473	1.000	19.61	
ANISOU	619	CG	PHE	77	2405	2530	2515	195	261	-516
ATOM	620	CD1	PHE	77	-9.966	22.594	56.395	1.000	22.27	
ANISOU	620	CD1	PHE	77	2514	3523	2426	431	-23	-527
ATOM	621	CD2	PHE	77	-11.917	21.285	55.941	1.000	21.31	
ANISOU	621	CD2	PHE	77	3282	2070	2743	36	615	-288
ATOM	622	CE1	PHE	77	-10.116	22.294	57.742	1.000	21.05	
ANISOU	622	CE1	PHE	77	2719	2768	2510	171	221	-339
ATOM	623	CE2	PHE	77	-12.079	20.991	57.300	1.000	25.09	
ANISOU	623	CE2	PHE	77	2967	4120	2447	-501	625	-826
ATOM	624	CZ	PHE	77	-11.175	21.523	58.207	1.000	23.79	
ANISOU	624	CZ	PHE	77	2263	3681	3095	-1	376	-756
ATOM	625	N	THR	78	-9.022	19.631	54.490	1.000	17.64	
ANISOU	625	N	THR	78	1616	2161	2925	37	336	1
ATOM	626	CA	THR	78	-9.296	18.279	54.983	1.000	18.12	
ANISOU	626	CA	THR	78	1926	2243	2717	-157	624	-28
ATOM	627	C	THR	78	-9.291	18.316	56.505	1.000	18.66	
ANISOU	627	C	THR	78	2120	2308	2663	-367	519	-288
ATOM	628	O	THR	78	-8.335	18.821	57.095	1.000	21.42	
ANISOU	628	O	THR	78	2158	2883	3098	-432	90	177
ATOM	629	CB	THR	78	-8.252	17.242	54.521	1.000	21.00	
ANISOU	629	CB	THR	78	2973	2067	2939	113	428	-574
ATOM	630	OG1	THR	78	-8.027	17.392	53.104	1.000	21.18	
ANISOU	630	OG1	THR	78	2544	2671	2833	160	317	-773
ATOM	631	CG2	THR	78	-8.735	15.832	54.800	1.000	26.65	
ANISOU	631	CG2	THR	78	3759	2227	4141	-275	853	-618
ATOM	632	N	GLY	79	-10.311	17.804	57.181	1.000	20.36	
ANISOU	632	N	GLY	79	2669	2379	2690	-670	630	-144
ATOM	633	CA	GLY	79	-10.344	17.679	58.623	1.000	25.96	
ANISOU	633	CA	GLY	79	3871	3249	2745	-790	576	375
ATOM	634	C	GLY	79	-10.029	16.238	59.039	1.000	39.70	
ANISOU	634	C	GLY	79	6407	3542	5135	-1658	-1944	1511
ATOM	635	O	GLY	79	-10.623	15.303	58.491	1.000	31.02	
ANISOU	635	O	GLY	79	4327	3187	4272	-404	419	-75
ATOM	636	N	LEU	80	-9.069	16.055	59.936	1.000	36.07	
ANISOU	636	N	LEU	80	4380	4536	4788	1381	-564	-835
ATOM	637	CA	LEU	80	-8.634	14.713	60.340	1.000	32.52	
ANISOU	637	CA	LEU	80	3640	4083	4632	611	-502	-898
ATOM	638	C	LEU	80	-9.131	14.311	61.716	1.000	39.82	
ANISOU	638	C	LEU	80	5051	4652	5428	-128	418	-538
ATOM	639	O	LEU	80	-9.998	14.963	62.305	1.000	37.05	
ANISOU	639	O	LEU	80	5057	3807	5213	-292	666	87
ATOM	640	CB	LEU	80	-7.122	14.580	60.265	1.000	38.36	
ANISOU	640	CB	LEU	80	3821	5456	5299	1568	-33	-1406
ATOM	641	CG	LEU	80	-6.488	14.753	58.883	1.000	38.27	

- 34 -

ANISOU	641	CG	LEU	80	3714	5900	4926	725	-288	-2588
ATOM	642	CD1	LEU	80	-5.007	14.359	58.948	1.000	45.41	
ANISOU	642	CD1	LEU	80	2579	8505	6170	-1092	-76	37
ATOM	643	CD2	LEU	80	-7.170	13.856	57.854	1.000	40.75	
ANISOU	643	CD2	LEU	80	4296	5601	5587	872	-1965	-1793
ATOM	644	N	SER	98	-6.459	17.442	63.930	1.000	36.72	
ANISOU	644	N	SER	98	3404	6429	4118	-2114	-698	1948
ATOM	645	CA	SER	98	-5.629	17.877	62.824	1.000	39.59	
ANISOU	645	CA	SER	98	6031	5376	3635	-449	383	2177
ATOM	646	C	SER	98	-6.402	18.372	61.610	1.000	29.89	
ANISOU	646	C	SER	98	3806	3509	4040	141	640	1204
ATOM	647	O	SER	98	-7.474	17.856	61.304	1.000	38.27	
ANISOU	647	O	SER	98	4936	4300	5303	-1107	395	885
ATOM	648	CB	SER	98	-4.694	16.739	62.358	1.000	44.06	
ANISOU	648	CB	SER	98	3175	7425	6141	633	-753	2704
ATOM	649	OG	SER	98	-3.672	17.368	61.583	1.000	46.84	
ANISOU	649	OG	SER	98	3497	6502	7797	95	-408	2418
ATOM	650	N	MET	99	-5.829	19.317	60.869	1.000	28.56	
ANISOU	650	N	MET	99	5029	3458	2365	-1080	-550	546
ATOM	651	CA	MET	99	-6.426	19.941	59.700	1.000	21.44	
ANISOU	651	CA	MET	99	2284	3549	2315	-182	157	132
ATOM	652	C	MET	99	-5.376	20.229	58.624	1.000	19.16	
ANISOU	652	C	MET	99	2306	2592	2382	-433	60	137
ATOM	653	O	MET	99	-4.232	20.575	58.930	1.000	23.34	
ANISOU	653	O	MET	99	2489	3920	2460	-773	225	-410
ATOM	654	CB	MET	99	-7.164	21.209	60.105	1.000	25.20	
ANISOU	654	CB	MET	99	3172	3375	3028	-572	661	-547
ATOM	655	CG	MET	99	-8.481	20.965	60.872	1.000	25.85	
ANISOU	655	CG	MET	99	3172	3862	2787	-275	739	-782
ATOM	656	SD	MET	99	-9.251	22.517	61.389	1.000	32.21	
ANISOU	656	SD	MET	99	4405	3750	4083	-133	1580	-568
ATOM	657	CE	MET	99	-8.884	22.461	63.145	1.000	76.12	
ANISOU	657	CE	MET	99	14782	11538	2603	-3321	3478	-3241
ATOM	658	N	CYS	100	-5.778	20.094	57.361	1.000	18.85	
ANISOU	658	N	CYS	100	2434	2443	2285	-160	93	194
ATOM	659	CA	CYS	100	-4.868	20.333	56.234	1.000	18.55	
ANISOU	659	CA	CYS	100	2251	2380	2418	92	127	236
ATOM	660	C	CYS	100	-5.496	21.312	55.228	1.000	16.26	
ANISOU	660	C	CYS	100	1826	2031	2321	110	329	2
ATOM	661	O	CYS	100	-6.728	21.308	55.071	1.000	17.69	
ANISOU	661	O	CYS	100	1741	2395	2586	-69	154	-104
ATOM	662	CB	CYS	100	-4.604	18.982	55.545	1.000	18.46	
ANISOU	662	CB	CYS	100	2822	2081	2111	98	118	511
ATOM	663	SG	CYS	100	-3.243	18.974	54.329	1.000	22.76	
ANISOU	663	SG	CYS	100	2622	2968	3058	307	391	10
ATOM	664	N	TYR	101	-4.697	22.069	54.498	1.000	17.49	
ANISOU	664	N	TYR	101	1839	2473	2332	46	291	224
ATOM	665	CA	TYR	101	-5.117	22.874	53.373	1.000	15.38	
ANISOU	665	CA	TYR	101	1946	1939	1960	-50	90	-262
ATOM	666	C	TYR	101	-4.102	22.594	52.245	1.000	13.65	
ANISOU	666	C	TYR	101	1676	1543	1967	-2	-123	-151
ATOM	667	O	TYR	101	-2.896	22.629	52.475	1.000	15.95	
ANISOU	667	O	TYR	101	1611	2231	2217	-43	-232	-212
ATOM	668	CB	TYR	101	-5.122	24.382	53.739	1.000	19.02	
ANISOU	668	CB	TYR	101	2816	2082	2328	234	48	-519
ATOM	669	CG	TYR	101	-5.617	25.109	52.498	1.000	17.85	
ANISOU	669	CG	TYR	101	2084	1895	2804	18	-26	-231
ATOM	670	CD1	TYR	101	-6.964	25.134	52.171	1.000	18.25	
ANISOU	670	CD1	TYR	101	2042	1596	3298	29	28	-496
ATOM	671	CD2	TYR	101	-4.730	25.778	51.658	1.000	17.77	
ANISOU	671	CD2	TYR	101	2037	1611	3106	-46	-125	-127

- 35 -

ATOM 672 CE1 TYR 101 -7.406 25.796 51.036 1.000 19.63
 ANISOU 672 CE1 TYR 101 1977 1776 3704 88 -241 -22 1
 ATOM 673 CE2 TYR 101 -5.147 26.386 50.478 1.000 20.46
 ANISOU 673 CE2 TYR 101 2060 2608 3108 239 40 18 2
 ATOM 674 CZ TYR 101 -6.504 26.392 50.166 1.000 20.29
 ANISOU 674 CZ TYR 101 2187 2397 3127 -73 -353 -26 0
 ATOM 675 OH TYR 101 -6.932 26.995 49.000 1.000 23.34
 ANISOU 675 OH TYR 101 2790 2555 3523 -3 -641 5 2
 ATOM 676 N SER 102 -4.648 22.210 51.097 1.000 14.60
 ANISOU 676 N SER 102 1618 1890 2041 -61 -109 -47 7
 ATOM 677 CA SER 102 -3.797 21.792 49.980 1.000 14.52
 ANISOU 677 CA SER 102 1684 1802 2030 -108 62 -27 6
 ATOM 678 C SER 102 -4.011 22.670 48.747 1.000 14.99
 ANISOU 678 C SER 102 1545 1790 2361 -296 -41 2 1
 ATOM 679 O SER 102 -5.167 23.105 48.477 1.000 16.73
 ANISOU 679 O SER 102 1589 2342 2425 2 128 -3
 ATOM 680 CB SER 102 -4.163 20.340 49.593 1.000 13.82
 ANISOU 680 CB SER 102 1692 1548 2013 174 9 -13 8
 ATOM 681 OG SER 102 -3.996 19.476 50.720 1.000 16.06
 ANISOU 681 OG SER 102 1886 2066 2153 97 -121 6 3
 ATOM 682 N MET 103 -2.978 22.775 47.920 1.000 14.47
 ANISOU 682 N MET 103 1568 1724 2206 51 -59 15 2
 ATOM 683 CA MET 103 -3.102 23.552 46.687 1.000 16.58
 ANISOU 683 CA MET 103 2194 1933 2173 331 -74 25 3
 ATOM 684 C MET 103 -2.150 23.013 45.608 1.000 14.41
 ANISOU 684 C MET 103 1598 1793 2083 -202 -210 6 3
 ATOM 685 O MET 103 -1.157 22.347 45.920 1.000 16.24
 ANISOU 685 O MET 103 1527 2384 2259 -61 -23 46 8
 ATOM 686 CB MET 103 -2.716 25.004 46.835 1.000 28.78
 ANISOU 686 CB MET 103 6537 1318 3081 859 -207 36 6
 ATOM 687 CG MET 103 -3.258 25.986 47.801 1.000 22.60
 ANISOU 687 CG MET 103 2531 2157 3900 -161 -57 -29 1
 ATOM 688 SD MET 103 -2.338 27.505 47.506 1.000 20.60
 ANISOU 688 SD MET 103 2499 1927 3400 -4 -164 -22 6
 ATOM 689 CE MET 103 -2.587 27.945 45.804 1.000 21.63
 ANISOU 689 CE MET 103 2319 2601 3300 308 209 -23 6
 ATOM 690 N GLY 104 -2.439 23.430 44.378 1.000 15.44
 ANISOU 690 N GLY 104 1468 2228 2169 -68 -120 16 4
 ATOM 691 CA GLY 104 -1.511 23.199 43.276 1.000 16.13
 ANISOU 691 CA GLY 104 1688 2202 2241 42 65 46 9
 ATOM 692 C GLY 104 -1.583 24.355 42.294 1.000 15.76
 ANISOU 692 C GLY 104 1706 1997 2286 -32 -194 38 8
 ATOM 693 O GLY 104 -1.987 25.478 42.653 1.000 19.06
 ANISOU 693 O GLY 104 1953 2032 3256 -71 144 33 3
 ATOM 694 N THR 105 -1.151 24.092 41.054 1.000 16.73
 ANISOU 694 N THR 105 1685 2385 2287 -375 -55 51 5
 ATOM 695 CA THR 105 -1.115 25.205 40.094 1.000 17.06
 ANISOU 695 CA THR 105 1725 2390 2369 -231 -148 57 7
 ATOM 696 C THR 105 -2.513 25.631 39.635 1.000 19.55
 ANISOU 696 C THR 105 1768 1817 3842 -160 -346 52 5
 ATOM 697 O THR 105 -2.680 26.703 39.059 1.000 22.41
 ANISOU 697 O THR 105 2262 2116 4136 -119 -520 84 2
 ATOM 698 CB THR 105 -0.301 24.857 38.840 1.000 17.57
 ANISOU 698 CB THR 105 1759 2877 2038 -394 -343 37 7
 ATOM 699 OG1 THR 105 -0.865 23.675 38.217 1.000 18.66
 ANISOU 699 OG1 THR 105 2035 2449 2607 -140 -458 41 6
 ATOM 700 CG2 THR 105 1.155 24.590 39.178 1.000 18.95
 ANISOU 700 CG2 THR 105 1748 2853 2601 -105 -248 29 6
 ATOM 701 N ALA 106 -3.507 24.751 39.741 1.000 16.52
 ANISOU 701 N ALA 106 1596 2293 2389 -180 -1 29 8
 ATOM 702 CA ALA 106 -4.846 25.035 39.218 1.000 16.59

- 36 -

ANISOU	702	CA	ALA	106	1692	1952	2660	-214	-209	2	4	3	
ATOM	703	C	ALA	106	-5.848	24.142	39.923	1.000	17.52				
ANISOU	703	C	ALA	106	1651	1821	3186	26	-66	5	5	5	
ATOM	704	O	ALA	106	-5.479	23.323	40.805	1.000	17.88				
ANISOU	704	O	ALA	106	2038	2087	2668	59	-51	3	8	8	
ATOM	705	CB	ALA	106	-4.862	24.838	37.713	1.000	20.31				
ANISOU	705	CB	ALA	106	2331	2764	2620	-197	-403	4	4	0	
ATOM	706	N	ASP	107	-7.149	24.329	39.717	1.000	18.00				
ANISOU	706	N	ASP	107	1576	2208	3057	-77	-120	4	9		
ATOM	707	CA	ASP	107	-8.217	23.535	40.344	1.000	17.46				
ANISOU	707	CA	ASP	107	1563	2191	2881	-83	-472	3	6	3	
ATOM	708	C	ASP	107	-8.173	23.753	41.859	1.000	17.74				
ANISOU	708	C	ASP	107	1825	2044	2869	447	-269	3	6	2	
ATOM	709	O	ASP	107	-8.458	22.854	42.650	1.000	18.95				
ANISOU	709	O	ASP	107	1994	2230	2974	167	-133	4	0	2	
ATOM	710	CB	ASP	107	-8.089	22.044	39.990	1.000	19.62				
ANISOU	710	CB	ASP	107	2213	2300	2942	-394	-727	1	7	3	
ATOM	711	CG	ASP	107	-8.370	21.842	38.508	1.000	20.81				
ANISOU	711	CG	ASP	107	1952	3093	2862	-138	-532	-	1	4	
ATOM	712	OD1	ASP	107	-9.369	22.369	37.976	1.000	25.84				
ANISOU	712	OD1	ASP	107	2524	3967	3327	222	-1149	-	2	4	0
ATOM	713	OD2	ASP	107	-7.544	21.168	37.844	1.000	25.86				
ANISOU	713	OD2	ASP	107	3314	2989	3523	391	-91	-	8	9	
ATOM	714	N	ASN	108	-7.893	24.962	42.298	1.000	18.18				
ANISOU	714	N	ASN	108	2049	2075	2786	509	189	1	5	3	
ATOM	715	CA	ASN	108	-7.831	25.263	43.740	1.000	17.10				
ANISOU	715	CA	ASN	108	1804	1977	2715	266	291	3	2	7	
ATOM	716	C	ASN	108	-9.158	25.716	44.314	1.000	17.11				
ANISOU	716	C	ASN	108	1705	2061	2734	367	44	1	4	9	
ATOM	717	O	ASN	108	-10.103	26.086	43.604	1.000	20.72				
ANISOU	717	O	ASN	108	2066	2377	3430	759	-248	2	4	5	
ATOM	718	CB	ASN	108	-6.799	26.379	43.969	1.000	19.90				
ANISOU	718	CB	ASN	108	1770	2308	3483	186	298	-	1	7	1
ATOM	719	CG	ASN	108	-5.400	25.862	43.717	1.000	17.24				
ANISOU	719	CG	ASN	108	1709	2212	2628	200	68	1	8	4	
ATOM	720	OD1	ASN	108	-4.986	24.850	44.277	1.000	17.42				
ANISOU	720	OD1	ASN	108	2003	1984	2631	109	11	-	6	2	
ATOM	721	ND2	ASN	108	-4.644	26.487	42.834	1.000	18.41				
ANISOU	721	ND2	ASN	108	2083	2326	2587	-82	300	-	1	8	
ATOM	722	N	LEU	109	-9.308	25.509	45.607	1.000	18.09				
ANISOU	722	N	LEU	109	1795	2294	2786	349	344	1	0		
ATOM	723	CA	LEU	109	-10.532	25.803	46.369	1.000	19.11				
ANISOU	723	CA	LEU	109	1763	2200	3296	14	476	-	5	9	8
ATOM	724	C	LEU	109	-10.169	26.790	47.457	1.000	17.40				
ANISOU	724	C	LEU	109	1682	1937	2990	251	129	-	2	0	7
ATOM	725	O	LEU	109	-9.443	26.423	48.395	1.000	21.18				
ANISOU	725	O	LEU	109	2443	1922	3684	174	-520	2			
ATOM	726	CB	LEU	109	-11.100	24.504	46.940	1.000	17.10				
ANISOU	726	CB	LEU	109	1888	2142	2469	199	426	-	6	3	0
ATOM	727	CG	LEU	109	-11.520	23.425	45.944	1.000	18.07				
ANISOU	727	CG	LEU	109	2515	1943	2409	190	-198	-	3	6	3
ATOM	728	CD1	LEU	109	-11.895	22.124	46.654	1.000	20.06				
ANISOU	728	CD1	LEU	109	2842	2406	2375	-331	-175	-	2	0	0
ATOM	729	CD2	LEU	109	-12.630	23.908	45.035	1.000	25.24				
ANISOU	729	CD2	LEU	109	3481	2892	3217	306	-992	-	1	1	1
ATOM	730	N	PHE	110	-10.609	28.036	47.313	1.000	17.25				
ANISOU	730	N	PHE	110	1584	1926	3045	272	184	-	1	3	2
ATOM	731	CA	PHE	110	-10.235	29.071	48.277	1.000	18.20				
ANISOU	731	CA	PHE	110	1751	1816	3346	169	221	-	1	6	0
ATOM	732	C	PHE	110	-11.409	29.567	49.106	1.000	19.93				
ANISOU	732	C	PHE	110	2077	1609	3886	71	650	-	3	3	5

- 37 -

ATOM	733	O	PHE	110	-12.433	29.948	48.494	1.000	24.64
ANISOU	733	O	PHE	110	2051	2461	4851	612	328 -779
ATOM	734	CB	PHE	110	-9.607	30.243	47.520	1.000	19.92
ANISOU	734	CB	PHE	110	2367	1876	3324	224	619 -93
ATOM	735	CG	PHE	110	-8.380	29.986	46.688	1.000	19.47
ANISOU	735	CG	PHE	110	2009	2209	3179	-321	327 -791
ATOM	736	CD1	PHE	110	-7.177	29.680	47.287	1.000	20.59
ANISOU	736	CD1	PHE	110	2071	2080	3674	-274	236 -331
ATOM	737	CD2	PHE	110	-8.437	30.035	45.299	1.000	20.19
ANISOU	737	CD2	PHE	110	2557	1914	3200	112	543 -289
ATOM	738	CE1	PHE	110	-6.034	29.454	46.559	1.000	21.06
ANISOU	738	CE1	PHE	110	2020	2309	3673	-386	165 -622
ATOM	739	CE2	PHE	110	-7.277	29.811	44.547	1.000	20.77
ANISOU	739	CE2	PHE	110	2495	2138	3257	197	504 -398
ATOM	740	CZ	PHE	110	-6.081	29.518	45.175	1.000	22.42
ANISOU	740	CZ	PHE	110	2747	2092	3678	531	339 -357
ATOM	741	N	PRO	111	-11.238	29.718	50.416	1.000	22.11
ANISOU	741	N	PRO	111	2250	2153	3996	-72	871 -620
ATOM	742	CA	PRO	111	-12.287	30.389	51.195	1.000	28.23
ANISOU	742	CA	PRO	111	3895	2210	4621	698	1514 -671
ATOM	743	C	PRO	111	-12.333	31.866	50.784	1.000	30.57
ANISOU	743	C	PRO	111	4528	2026	5061	410	410 -1041
ATOM	744	O	PRO	111	-11.390	32.340	50.115	1.000	31.71
ANISOU	744	O	PRO	111	4040	2236	5774	-179	-597 -12
ATOM	745	CB	PRO	111	-11.799	30.250	52.627	1.000	33.20
ANISOU	745	CB	PRO	111	5609	2702	4303	671	1671 -790
ATOM	746	CG	PRO	111	-10.646	29.326	52.647	1.000	26.04
ANISOU	746	CG	PRO	111	2742	3316	3835	-931	1324 -192
ATOM	747	CD	PRO	111	-10.161	29.149	51.230	1.000	22.15
ANISOU	747	CD	PRO	111	2587	2307	3522	-471	541 -623
ATOM	748	N	SER	112	-13.337	32.641	51.150	1.000	42.13
ANISOU	748	N	SER	112	7176	2716	6115	2074	1731 -526
ATOM	749	CA	SER	112	-13.368	34.026	50.672	1.000	44.05
ANISOU	749	CA	SER	112	6799	2255	7684	1107	-485 -826
ATOM	750	C	SER	112	-13.262	34.157	49.149	1.000	68.28
ANISOU	750	C	SER	112	13632	4498	7812	-1855	-2077 1301
ATOM	751	O	SER	112	-12.347	34.825	48.646	1.000	95.18
ANISOU	751	O	SER	112	15991	11425	8747	-4337	-70 1985
ATOM	752	CB	SER	112	-12.493	35.069	51.349	1.000	39.31
ANISOU	752	CB	SER	112	2247	4535	8153	580	1662 -1437
ATOM	753	OG	SER	112	-11.474	34.624	52.213	1.000	37.49
ANISOU	753	OG	SER	112	7213	2453	4579	806	747 -1152
ATOM	754	N	ASP	114	-9.515	37.322	49.945	1.000	36.40
ANISOU	754	N	ASP	114	3476	2118	8237	1254	403 1484
ATOM	755	CA	ASP	114	-8.205	37.586	50.600	1.000	30.79
ANISOU	755	CA	ASP	114	3503	2856	5340	1229	1240 996
ATOM	756	C	ASP	114	-7.242	36.402	50.648	1.000	26.16
ANISOU	756	C	ASP	114	2581	2404	4955	601	1114 804
ATOM	757	O	ASP	114	-6.031	36.458	50.338	1.000	25.45
ANISOU	757	O	ASP	114	2302	2503	4866	-43	602 131
ATOM	758	CB	ASP	114	-8.595	37.874	52.075	1.000	43.68
ANISOU	758	CB	ASP	114	7509	2783	6304	1157	2727 -210
ATOM	759	CG	ASP	114	-7.391	38.386	52.835	1.000	46.96
ANISOU	759	CG	ASP	114	9259	3225	5359	2517	519 107
ATOM	760	OD1	ASP	114	-6.487	38.959	52.189	1.000	83.49
ANISOU	760	OD1	ASP	114	13724	9866	8132	-6354	650 -3056
ATOM	761	OD2	ASP	114	-7.370	38.262	54.071	1.000	113.59
ANISOU	761	OD2	ASP	114	27880	10550	4730	-6984	-159 -2575
ATOM	762	N	PHE	115	-7.831	35.323	51.153	1.000	22.32
ANISOU	762	N	PHE	115	2620	2062	3799	204	954 -114
ATOM	763	CA	PHE	115	-7.115	34.026	51.183	1.000	22.69

- 38 -

ANISOU	763	CA	PHE	115	2765	1909	3947	118	1093	-187
ATOM	764	C	PHE	115	-6.502	33.754	49.816	1.000	21.49	
ANISOU	764	C	PHE	115	2146	2316	3702	305	559	-255
ATOM	765	O	PHE	115	-5.328	33.362	49.758	1.000	20.51	
ANISOU	765	O	PHE	115	2153	2011	3627	323	488	-158
ATOM	766	CB	PHE	115	-8.096	32.928	51.638	1.000	20.76	
ANISOU	766	CB	PHE	115	2369	1946	3574	-3	563	-473
ATOM	767	CG	PHE	115	-7.496	31.590	51.998	1.000	20.23	
ANISOU	767	CG	PHE	115	2369	1854	3463	-155	629	-377
ATOM	768	CD1	PHE	115	-6.915	30.756	51.041	1.000	20.35	
ANISOU	768	CD1	PHE	115	2572	1786	3372	-195	112	-756
ATOM	769	CD2	PHE	115	-7.474	31.152	53.309	1.000	21.11	
ANISOU	769	CD2	PHE	115	2802	1932	3287	-113	17	-689
ATOM	770	CE1	PHE	115	-6.351	29.538	51.325	1.000	21.09	
ANISOU	770	CE1	PHE	115	2502	1728	3784	-295	471	-538
ATOM	771	CE2	PHE	115	-6.938	29.901	53.623	1.000	27.40	
ANISOU	771	CE2	PHE	115	5012	1955	3445	444	43	-572
ATOM	772	CZ	PHE	115	-6.332	29.110	52.655	1.000	24.92	
ANISOU	772	CZ	PHE	115	3356	1889	4222	50	1519	221
ATOM	773	N	GLU	116	-7.301	33.768	48.757	1.000	21.64	
ANISOU	773	N	GLU	116	2396	1835	3990	338	261	-13
ATOM	774	CA	GLU	116	-6.750	33.424	47.444	1.000	20.90	
ANISOU	774	CA	GLU	116	2235	1965	3742	224	74	116
ATOM	775	C	GLU	116	-5.550	34.262	47.054	1.000	20.32	
ANISOU	775	C	GLU	116	1978	1899	3845	439	-108	448
ATOM	776	O	GLU	116	-4.544	33.679	46.604	1.000	20.18	
ANISOU	776	O	GLU	116	2209	2147	3312	424	73	139
ATOM	777	CB	GLU	116	-7.851	33.561	46.385	1.000	24.22	
ANISOU	777	CB	GLU	116	2425	2638	4139	-467	-237	519
ATOM	778	CG	GLU	116	-7.339	33.331	44.980	1.000	23.27	
ANISOU	778	CG	GLU	116	2425	2465	3952	-7	-494	750
ATOM	779	CD	GLU	116	-8.401	33.273	43.910	1.000	25.02	
ANISOU	779	CD	GLU	116	2695	2703	4107	-510	-739	1509
ATOM	780	OE1	GLU	116	-9.617	33.306	44.207	1.000	34.83	
ANISOU	780	OE1	GLU	116	2466	4606	6161	-203	-928	1566
ATOM	781	OE2	GLU	116	-8.001	33.030	42.763	1.000	40.92	
ANISOU	781	OE2	GLU	116	4389	7172	3988	-24	-968	693
ATOM	782	N	ARG	117	-5.549	35.571	47.300	1.000	20.60	
ANISOU	782	N	ARG	117	2299	1811	3718	382	-10	469
ATOM	783	CA	ARG	117	-4.374	36.374	46.866	1.000	22.65	
ANISOU	783	CA	ARG	117	2230	1791	4586	351	107	153
ATOM	784	C	ARG	117	-3.163	35.911	47.648	1.000	21.87	
ANISOU	784	C	ARG	117	2269	1865	4178	252	179	97
ATOM	785	O	ARG	117	-2.060	35.789	47.102	1.000	22.10	
ANISOU	785	O	ARG	117	2197	2270	3931	216	41	205
ATOM	786	CB	ARG	117	-4.682	37.861	47.105	1.000	29.47	
ANISOU	786	CB	ARG	117	2849	1691	6658	259	-555	-1
ATOM	787	CG	ARG	117	-3.485	38.815	47.046	1.000	40.24	
ANISOU	787	CG	ARG	117	3905	2567	8818	-819	-1330	-476
ATOM	788	CD	ARG	117	-3.745	40.160	47.716	1.000	52.75	
ANISOU	788	CD	ARG	117	4698	2848	12496	-595	-1653	-1669
ATOM	789	NE	ARG	117	-3.934	39.987	49.155	1.000	68.00	
ANISOU	789	NE	ARG	117	8247	4719	12872	422	1842	-3441
ATOM	790	CZ	ARG	117	-3.166	40.448	50.126	1.000	78.38	
ANISOU	790	CZ	ARG	117	13026	5658	11097	283	448	-2498
ATOM	791	NH1	ARG	117	-2.097	41.186	49.849	1.000	89.01	
ANISOU	791	NH1	ARG	117	14218	11488	8115	-3550	-6761	3577
ATOM	792	NH2	ARG	117	-3.479	40.189	51.391	1.000	82.58	
ANISOU	792	NH2	ARG	117	16575	2856	11947	2617	2551	-2095
ATOM	793	N	ILE	118	-3.334	35.759	48.954	1.000	21.70	
ANISOU	793	N	ILE	118	2319	1797	4127	311	271	-314

- 39 -

ATOM	794	CA	ILE	118	-2.206	35.425	49.810	1.000	20.99
ANISOU	794	CA	ILE	118	2546	1624	3805	408	294 - 470
ATOM	795	C	ILE	118	-1.596	34.073	49.475	1.000	18.79
ANISOU	795	C	ILE	118	2222	1534	3384	218	573 - 201
ATOM	796	O	ILE	118	-0.409	33.858	49.323	1.000	17.27
ANISOU	796	O	ILE	118	2194	1663	2707	283	351 - 136
ATOM	797	CB	ILE	118	-2.588	35.542	51.293	1.000	22.62
ANISOU	797	CB	ILE	118	2702	1997	3895	276	416 - 856
ATOM	798	CG1	ILE	118	-2.916	36.995	51.700	1.000	27.54
ANISOU	798	CG1	ILE	118	5077	1801	3587	503	768 - 401
ATOM	799	CG2	ILE	118	-1.552	34.940	52.206	1.000	23.59
ANISOU	799	CG2	ILE	118	3084	2274	3606	183	254 - 818
ATOM	800	CD1	ILE	118	-3.493	37.115	53.096	1.000	29.35
ANISOU	800	CD1	ILE	118	5212	2054	3885	558	1114 - 645
ATOM	801	N	TRP	119	-2.454	33.069	49.341	1.000	17.93
ANISOU	801	N	TRP	119	2378	1605	2828	147	-80 - 2'69
ATOM	802	CA	TRP	119	-2.035	31.688	49.103	1.000	16.57
ANISOU	802	CA	TRP	119	2126	1538	2630	152	-25 - 16
ATOM	803	C	TRP	119	-1.575	31.476	47.676	1.000	16.98
ANISOU	803	C	TRP	119	2126	1723	2604	269	-91 - 51
ATOM	804	O	TRP	119	-0.700	30.640	47.455	1.000	17.58
ANISOU	804	O	TRP	119	1892	1674	3113	135	181 6 3
ATOM	805	CB	TRP	119	-3.127	30.690	49.591	1.000	18.32
ANISOU	805	CB	TRP	119	2156	1789	3014	-34	5 - 7
ATOM	806	CG	TRP	119	-2.934	30.457	51.082	1.000	18.27
ANISOU	806	CG	TRP	119	2208	1711	3025	86	349 5 6
ATOM	807	CD1	TRP	119	-3.354	31.273	52.103	1.000	20.36
ANISOU	807	CD1	TRP	119	2624	2029	3083	156	276 - 153
ATOM	808	CD2	TRP	119	-2.213	29.383	51.683	1.000	18.61
ANISOU	808	CD2	TRP	119	2049	2055	2967	134	263 110
ATOM	809	NE1	TRP	119	-2.955	30.773	53.323	1.000	20.55
ANISOU	809	NE1	TRP	119	2471	2229	3109	92	266 - 106
ATOM	810	CE2	TRP	119	-2.260	29.603	53.073	1.000	20.21
ANISOU	810	CE2	TRP	119	2529	2258	2893	180	754 297
ATOM	811	CE3	TRP	119	-1.576	28.258	51.147	1.000	18.29
ANISOU	811	CE3	TRP	119	2258	1714	2977	42	-70 - 20
ATOM	812	CZ2	TRP	119	-1.636	28.728	53.981	1.000	21.97
ANISOU	812	CZ2	TRP	119	2876	2526	2945	384	51 - 106
ATOM	813	CZ3	TRP	119	-0.968	27.375	52.045	1.000	19.35
ANISOU	813	CZ3	TRP	119	2576	2028	2750	187	415 299
ATOM	814	CH2	TRP	119	-1.026	27.618	53.442	1.000	21.67
ANISOU	814	CH2	TRP	119	3033	2379	2823	350	250 97
ATOM	815	N	THR	120	-2.129	32.192	46.701	1.000	16.93
ANISOU	815	N	THR	120	2023	1833	2577	122	-112 18
ATOM	816	CA	THR	120	-1.598	32.086	45.342	1.000	17.85
ANISOU	816	CA	THR	120	1915	2469	2398	222	-371 - 324
ATOM	817	C	THR	120	-0.169	32.587	45.288	1.000	17.15
ANISOU	817	C	THR	120	2031	1855	2629	241	-155 192
ATOM	818	O	THR	120	0.700	31.960	44.674	1.000	18.67
ANISOU	818	O	THR	120	1996	1887	3212	389	-131 177
ATOM	819	CB	THR	120	-2.487	32.865	44.344	1.000	18.10
ANISOU	819	CB	THR	120	1951	2204	2720	28	-93 345
ATOM	820	OG1	THR	120	-3.773	32.238	44.284	1.000	20.49
ANISOU	820	OG1	THR	120	1807	2801	3179	59	-363 558
ATOM	821	CG2	THR	120	-1.919	32.803	42.933	1.000	22.46
ANISOU	821	CG2	THR	120	2438	3266	2830	475	118 705
ATOM	822	N	GLN	121	0.094	33.708	45.956	1.000	18.62
ANISOU	822	N	GLN	121	2180	1657	3237	123	-94 213
ATOM	823	CA	GLN	121	1.466	34.232	45.993	1.000	18.15
ANISOU	823	CA	GLN	121	2077	1698	3119	77	96 520
ATOM	824	C	GLN	121	2.412	33.284	46.718	1.000	17.04

- 40 -

ANISOU	824	C	GLN	121	2022	1431	3019	192	234	2 2 3
ATOM	825	O	GLN	121	3.510	33.047	46.270	1.000	19.32	
ANISOU	825	O	GLN	121	1894	1800	3645	93	246	1 2 9
ATOM	826	CB	GLN	121	1.490	35.579	46.756	1.000	22.90	
ANISOU	826	CB	GLN	121	2520	1479	4702	327	-812	2 7 1
ATOM	827	CG	GLN	121	2.888	36.159	46.871	1.000	27.04	
ANISOU	827	CG	GLN	121	2949	2062	5262	-346	-400	1 3 2
ATOM	828	CD	GLN	121	3.530	36.511	45.535	1.000	31.94	
ANISOU	828	CD	GLN	121	3307	2733	6097	983	1031	9 9
ATOM	829	OE1	GLN	121	4.660	36.085	45.247	1.000	62.76	
ANISOU	829	OE1	GLN	121	3009	9570	11267	1758	2366	2 0 2 9
ATOM	830	NE2	GLN	121	2.859	37.306	44.716	1.000	55.89	
ANISOU	830	NE2	GLN	121	6516	7728	6993	2815	1745	3 2 4 9
ATOM	831	N	TYR	122	1.997	32.791	47.871	1.000	16.87	
ANISOU	831	N	TYR	122	2389	1518	2501	71	-161	- 5 4
ATOM	832	CA	TYR	122	2.795	31.881	48.683	1.000	17.97	
ANISOU	832	CA	TYR	122	2564	1600	2666	176	-224	- 5 6
ATOM	833	C	TYR	122	3.080	30.600	47.909	1.000	16.83	
ANISOU	833	C	TYR	122	1870	1460	3065	-31	-57	- 9 8
ATOM	834	O	TYR	122	4.224	30.129	47.823	1.000	17.67	
ANISOU	834	O	TYR	122	1891	1952	2872	189	-220	1 2 6
ATOM	835	CB	TYR	122	2.018	31.522	49.960	1.000	18.01	
ANISOU	835	CB	TYR	122	2526	1821	2495	2	-325	- 5 5
ATOM	836	CG	TYR	122	2.753	30.619	50.898	1.000	17.89	
ANISOU	836	CG	TYR	122	2332	1695	2769	255	-147	- 5 1
ATOM	837	CD1	TYR	122	4.058	30.901	51.323	1.000	21.71	
ANISOU	837	CD1	TYR	122	2883	2101	3267	-257	-913	3 4
ATOM	838	CD2	TYR	122	2.107	29.496	51.415	1.000	21.29	
ANISOU	838	CD2	TYR	122	2428	2026	3634	128	-267	4 6 8
ATOM	839	CE1	TYR	122	4.680	30.037	52.212	1.000	21.27	
ANISOU	839	CE1	TYR	122	2681	2045	3356	140	-725	- 2 1 0
ATOM	840	CE2	TYR	122	2.746	28.637	52.290	1.000	24.50	
ANISOU	840	CE2	TYR	122	3376	1876	4057	-292	-1163	5 0 6
ATOM	841	CZ	TYR	122	4.043	28.914	52.675	1.000	22.16	
ANISOU	841	CZ	TYR	122	3161	1881	3379	95	-909	- 1 2 8
ATOM	842	OH	TYR	122	4.699	28.079	53.566	1.000	23.72	
ANISOU	842	OH	TYR	122	3471	2398	3142	52	-1005	- 5 6
ATOM	843	N	PHE	123	2.074	30.023	47.253	1.000	16.21	
ANISOU	843	N	PHE	123	1794	1571	2793	49	-66	- 5 4
ATOM	844	CA	PHE	123	2.347	28.843	46.397	1.000	15.71	
ANISOU	844	CA	PHE	123	1622	1800	2548	34	-142	- 1 0 3
ATOM	845	C	PHE	123	3.378	29.188	45.337	1.000	15.96	
ANISOU	845	C	PHE	123	1681	1304	3078	42	90	3
ATOM	846	O	PHE	123	4.276	28.375	45.037	1.000	15.47	
ANISOU	846	O	PHE	123	1703	1437	2739	54	14	- 2 4
ATOM	847	CB	PHE	123	1.036	28.309	45.779	1.000	15.07	
ANISOU	847	CB	PHE	123	1460	1364	2904	209	-148	1
ATOM	848	CG	PHE	123	1.241	27.104	44.879	1.000	17.41	
ANISOU	848	CG	PHE	123	2090	1620	2906	-39	-179	- 2 3 8
ATOM	849	CD1	PHE	123	1.170	25.831	45.452	1.000	17.41	
ANISOU	849	CD1	PHE	123	1680	1439	3494	72	-119	- 2 5 5
ATOM	850	CD2	PHE	123	1.490	27.259	43.513	1.000	18.22	
ANISOU	850	CD2	PHE	123	1723	2331	2870	-96	-216	- 3 7 2
ATOM	851	CE1	PHE	123	1.419	24.740	44.636	1.000	19.15	
ANISOU	851	CE1	PHE	123	2112	1766	3397	212	-540	- 5 3 6
ATOM	852	CE2	PHE	123	1.722	26.144	42.717	1.000	19.63	
ANISOU	852	CE2	PHE	123	1901	2476	3083	-134	-261	- 6 3 2
ATOM	853	CZ	PHE	123	1.635	24.868	43.274	1.000	19.40	
ANISOU	853	CZ	PHE	123	1525	2424	3421	385	-529	- 4 9 0
ATOM	854	N	ASP	124	3.164	30.304	44.636	1.000	16.86	
ANISOU	854	N	ASP	124	1947	1466	2992	-23	-110	1 2 4

- 41 -

ATOM	855	CA	ASP	124	4.060	30.640	43.544	1.000	17.82
ANISOU	855	CA	ASP	124	2103	1747	2921	405	-24 3 1 4
ATOM	856	C	ASP	124	5.490	30.733	44.024	1.000	17.52
ANISOU	856	C	ASP	124	1999	1439	3219	181	94 8 9
ATOM	857	O	ASP	124	6.402	30.324	43.317	1.000	17.18
ANISOU	857	O	ASP	124	2086	1427	3015	34 181	1 7 7
ATOM	858	CB	AASP	124	3.639	31.997	42.942	0.534	21.77
ANISOU	858	CB	AASP	124	3475	2089	2706	642	-372 5 9 7
ATOM	859	CG	AASP	124	4.381	32.304	41.659	0.534	19.28
ANISOU	859	CG	AASP	124	2376	1982	2967	173	-553 4 9 5
ATOM	860	OD1	AASP	124	4.223	31.538	40.678	0.534	21.03
ANISOU	860	OD1	AASP	124	2189	2636	3164	-28	76 2 1
ATOM	861	OD2	AASP	124	5.068	33.348	41.639	0.534	24.96
ANISOU	861	OD2	AASP	124	3681	2052	3752	-296	-1067 8 8 9
ATOM	862	CB	BASP	124	3.632	31.975	42.908	0.466	19.67
ANISOU	862	CB	BASP	124	2559	1993	2923	1003	673 4 4 6
ATOM	863	CG	BASP	124	2.368	31.849	42.089	0.466	22.78
ANISOU	863	CG	BASP	124	3552	3217	1889	872	177 1 1 7 5
ATOM	864	OD1	BASP	124	2.021	30.781	41.545	0.466	27.78
ANISOU	864	OD1	BASP	124	2138	3932	4483	100	503 3 4 7
ATOM	865	OD2	BASP	124	1.703	32.893	41.902	0.466	29.73
ANISOU	865	OD2	BASP	124	3845	3804	3646	1239	-312 1 6 4 4
ATOM	866	N	ARG	125	5.669	31.416	45.153	1.000	16.65
ANISOU	866	N	ARG	125	1942	1350	3032	276	139 2 7 6
ATOM	867	CA	ARG	125	7.038	31.528	45.646	1.000	17.58
ANISOU	867	CA	ARG	125	1918	1819	2944	98 177	2 4 1
ATOM	868	C	ARG	125	7.662	30.188	45.992	1.000	17.38
ANISOU	868	C	ARG	125	1544	1777	3282	-42	40 2 7 3
ATOM	869	O	ARG	125	8.841	29.942	45.754	1.000	18.26
ANISOU	869	O	ARG	125	1639	1669	3631	-97	91 -2 3 3
ATOM	870	CB	ARG	125	7.062	32.468	46.851	1.000	20.45
ANISOU	870	CB	ARG	125	2219	2162	3387	-244	450 -2 7 4
ATOM	871	CG	ARG	125	6.860	33.916	46.344	1.000	28.23
ANISOU	871	CG	ARG	125	3178	2007	5542	147	666 -2 2 2
ATOM	872	CD	ARG	125	6.693	34.891	47.477	1.000	31.76
ANISOU	872	CD	ARG	125	3065	2279	6725	-628	1455 -9 9 3
ATOM	873	NE	ARG	125	6.496	36.221	46.932	1.000	40.81
ANISOU	873	NE	ARG	125	3332	2095	10080	-169	1790 -6 9 4
ATOM	874	CZ	ARG	125	5.970	37.229	47.628	1.000	43.42
ANISOU	874	CZ	ARG	125	4531	2891	9076	839	2072 -1 8 8
ATOM	875	NH1	ARG	125	5.551	37.025	48.866	1.000	38.62
ANISOU	875	NH1	ARG	125	3999	2858	7816	-858	61 -7 0 0
ATOM	876	NH2	ARG	125	5.858	38.382	47.006	1.000	42.11
ANISOU	876	NH2	ARG	125	5319	2652	8030	908	1627 -6 8 1
ATOM	877	N	GLN	126	6.884	29.282	46.557	1.000	15.28
ANISOU	877	N	GLN	126	1876	1527	2404	-70	13 -6 0
ATOM	878	CA	GLN	126	7.376	27.929	46.853	1.000	15.37
ANISOU	878	CA	GLN	126	1726	1625	2488	-54	-312 2 0
ATOM	879	C	GLN	126	7.649	27.150	45.578	1.000	14.21
ANISOU	879	C	GLN	126	1643	1268	2488	-75	-398 7 1
ATOM	880	O	GLN	126	8.682	26.462	45.496	1.000	15.36
ANISOU	880	O	GLN	126	1531	1554	2753	-37	-316 5 3
ATOM	881	CB	GLN	126	6.356	27.158	47.702	1.000	17.40
ANISOU	881	CB	GLN	126	2034	1313	3264	158	293 4 3
ATOM	882	CG	GLN	126	6.336	27.634	49.150	1.000	26.14
ANISOU	882	CG	GLN	126	4503	1690	3739	431	1908 -7 3 2
ATOM	883	CD	GLN	126	5.208	26.998	49.891	1.000	21.95
ANISOU	883	CD	GLN	126	2957	2670	2713	0	-123 1 0 2
ATOM	884	OE1	GLN	126	4.051	27.372	49.730	1.000	42.52
ANISOU	884	OE1	GLN	126	2994	5747	7416	-62	-1272 3 1 4 7
ATOM	885	NE2	GLN	126	5.524	26.003	50.691	1.000	28.32

- 42 -

ANISOU	885	NE2	GLN	126	2867	3971	3922	-184	-780	13	11
ATOM	886	N	TYR	127	6.797	27.287	44.574	1.000	14.52		
ANISOU	886	N	TYR	127	1629	1438	2448	-41	-373	-3	6
ATOM	887	CA	TYR	127	7.039	26.554	43.317	1.000	13.93		
ANISOU	887	CA	TYR	127	1563	1455	2277	-136	-234	15	0
ATOM	888	C	TYR	127	8.289	27.091	42.624	1.000	14.54		
ANISOU	888	C	TYR	127	1461	1318	2745	24	-195	19	0
ATOM	889	O	TYR	127	9.133	26.345	42.140	1.000	14.39		
ANISOU	889	O	TYR	127	1611	1580	2277	34	-252	9	
ATOM	890	CB	TYR	127	5.801	26.676	42.435	1.000	14.00		
ANISOU	890	CB	TYR	127	1510	1549	2258	29	-180	-7	0
ATOM	891	CG	TYR	127	5.752	25.795	41.202	1.000	12.33		
ANISOU	891	CG	TYR	127	1315	1037	2334	-34	-187	4	5
ATOM	892	CD1	TYR	127	6.483	24.626	41.024	1.000	14.05		
ANISOU	892	CD1	TYR	127	1810	1158	2371	7	-84	-8	
ATOM	893	CD2	TYR	127	4.837	26.086	40.206	1.000	15.71		
ANISOU	893	CD2	TYR	127	1936	1548	2484	55	-513	2	1
ATOM	894	CE1	TYR	127	6.382	23.829	39.899	1.000	13.10		
ANISOU	894	CE1	TYR	127	1450	999	2529	-101	-227	-6	2
ATOM	895	CE2	TYR	127	4.661	25.322	39.071	1.000	15.07		
ANISOU	895	CE2	TYR	127	1928	1620	2177	158	-342	19	7
ATOM	896	CZ	TYR	127	5.440	24.179	38.934	1.000	13.71		
ANISOU	896	CZ	TYR	127	1617	1348	2245	-146	-106	24	6
ATOM	897	OH	TYR	127	5.337	23.386	37.811	1.000	15.04		
ANISOU	897	OH	TYR	127	1682	1755	2279	-87	-60	5	3
ATOM	898	N	THR	128	8.467	28.412	42.616	1.000	14.69		
ANISOU	898	N	THR	128	1813	1324	2446	-154	-217	26	8
ATOM	899	CA	THR	128	9.673	28.984	42.011	1.000	14.67		
ANISOU	899	CA	THR	128	1867	1469	2238	-98	-32	19	5
ATOM	900	C	THR	128	10.921	28.552	42.736	1.000	14.68		
ANISOU	900	C	THR	128	1794	1318	2466	59	-123	-28	5
ATOM	901	O	THR	128	11.900	28.166	42.062	1.000	15.45		
ANISOU	901	O	THR	128	1715	1487	2667	-259	153	7	1
ATOM	902	CB	THR	128	9.572	30.544	42.069	1.000	16.02		
ANISOU	902	CB	THR	128	2043	1348	2695	-79	59	47	9
ATOM	903	OG1	THR	128	8.519	30.849	41.162	1.000	19.14		
ANISOU	903	OG1	THR	128	2226	2038	3008	195	-23	54	5
ATOM	904	CG2	THR	128	10.835	31.187	41.582	1.000	19.03		
ANISOU	904	CG2	THR	128	2107	1329	3793	125	311	61	8
ATOM	905	N	ALA	129	10.933	28.564	44.085	1.000	14.21		
ANISOU	905	N	ALA	129	1708	1266	2424	-137	-256	-18	1
ATOM	906	CA	ALA	129	12.108	28.110	44.836	1.000	15.08		
ANISOU	906	CA	ALA	129	1670	1435	2624	-118	-210	-22	5
ATOM	907	C	ALA	129	12.389	26.643	44.562	1.000	14.37		
ANISOU	907	C	ALA	129	1706	1299	2457	-159	-203	15	7
ATOM	908	O	ALA	129	13.552	26.238	44.445	1.000	14.10		
ANISOU	908	O	ALA	129	1758	1464	2137	-5	-244	-14	8
ATOM	909	CB	ALA	129	11.887	28.313	46.313	1.000	17.08		
ANISOU	909	CB	ALA	129	2132	1851	2506	-183	-514	-23	9
ATOM	910	N	SER	130	11.343	25.819	44.553	1.000	14.18		
ANISOU	910	N	SER	130	1884	1237	2267	-224	-257	17	3
ATOM	911	CA	SER	130	11.487	24.375	44.351	1.000	15.44		
ANISOU	911	CA	SER	130	1840	1219	2807	-115	-135	-7	
ATOM	912	C	SER	130	12.072	24.114	42.965	1.000	14.45		
ANISOU	912	C	SER	130	1345	1481	2665	78	-796	-20	9
ATOM	913	O	SER	130	13.037	23.329	42.807	1.000	14.43		
ANISOU	913	O	SER	130	1327	1382	2773	-74	-246	17	2
ATOM	914	CB	SER	130	10.120	23.677	44.663	1.000	17.54		
ANISOU	914	CB	SER	130	1555	1225	3884	-379	-647	12	6
ATOM	915	OG	SER	130	9.268	23.888	43.558	1.000	27.32		
ANISOU	915	OG	SER	130	2321	3168	4893	11	-1207	86	5

- 43 -

ATOM	916	N	ARG	131	11.555	24.772	41.909	1.000	14.47
ANISOU	916	N	ARG	131	1421	1448	2628	161	-384 -166
ATOM	917	CA	ARG	131	12.163	24.598	40.592	1.000	14.91
ANISOU	917	CA	ARG	131	1689	1452	2525	-4	-526 -341
ATOM	918	C	ARG	131	13.605	25.079	40.566	1.000	14.05
ANISOU	918	C	ARG	131	1772	1435	2132	-72	-381 -173
ATOM	919	O	ARG	131	14.448	24.438	39.912	1.000	15.14
ANISOU	919	O	ARG	131	1829	1658	2267	-109	-170 -230
ATOM	920	CB	ARG	131	11.349	25.316	39.514	1.000	15.77
ANISOU	920	CB	ARG	131	1720	1613	2660	-54	-493 -94
ATOM	921	CG	ARG	131	9.970	24.737	39.251	1.000	16.08
ANISOU	921	CG	ARG	131	1703	1695	2711	-13	-647 -141
ATOM	922	CD	ARG	131	9.326	25.390	38.017	1.000	26.56
ANISOU	922	CD	ARG	131	3589	2689	3813	-1037	-2156 745
ATOM	923	NE	ARG	131	9.327	26.831	37.918	1.000	25.91
ANISOU	923	NE	ARG	131	2856	2814	4174	-979	-1682 1413
ATOM	924	CZ	ARG	131	8.472	27.716	38.413	1.000	31.86
ANISOU	924	CZ	ARG	131	3546	2861	5697	-254	-1094 2201
ATOM	925	NH1	ARG	131	7.467	27.244	39.138	1.000	31.34
ANISOU	925	NH1	ARG	131	5127	3636	3144	-1474	-458 -115
ATOM	926	NH2	ARG	131	8.633	29.032	38.235	1.000	40.12
ANISOU	926	NH2	ARG	131	3500	2831	8912	-582	-1620 1802
ATOM	927	N	ALA	132	13.893	26.186	41.236	1.000	13.42
ANISOU	927	N	ALA	132	1683	1385	2033	-85	-652 -24
ATOM	928	CA	ALA	132	15.246	26.751	41.128	1.000	13.38
ANISOU	928	CA	ALA	132	1617	1443	2022	-16	-499 -79
ATOM	929	C	ALA	132	16.225	25.808	41.837	1.000	13.37
ANISOU	929	C	ALA	132	1398	1365	2316	-93	-253 154
ATOM	930	O	ALA	132	17.306	25.586	41.328	1.000	14.43
ANISOU	930	O	ALA	132	1459	1772	2251	-91	-240 106
ATOM	931	CB	ALA	132	15.275	28.084	41.859	1.000	16.52
ANISOU	931	CB	ALA	132	2019	1243	3014	-199	-366 -236
ATOM	932	N	VAL	133	15.893	25.248	42.996	1.000	13.62
ANISOU	932	N	VAL	133	1522	1515	2139	-63	-362 86
ATOM	933	CA	VAL	133	16.839	24.363	43.689	1.000	14.86
ANISOU	933	CA	VAL	133	1902	1566	2179	120	-491 -27
ATOM	934	C	VAL	133	16.923	23.073	42.890	1.000	15.04
ANISOU	934	C	VAL	133	1390	1633	2690	-9	-220 -218
ATOM	935	O	VAL	133	18.036	22.538	42.773	1.000	15.49
ANISOU	935	O	VAL	133	1442	1814	2630	63	-193 -99
ATOM	936	CB	VAL	133	16.545	24.170	45.187	1.000	14.61
ANISOU	936	CB	VAL	133	1528	1789	2234	-45	-391 210
ATOM	937	CG1	VAL	133	15.362	23.267	45.453	1.000	16.78
ANISOU	937	CG1	VAL	133	1544	2123	2708	-249	-437 -81
ATOM	938	CG2	VAL	133	17.766	23.650	45.950	1.000	16.51
ANISOU	938	CG2	VAL	133	1769	1942	2561	-61	-831 64
ATOM	939	N	ALA	134	15.840	22.583	42.270	1.000	13.73
ANISOU	939	N	ALA	134	1605	1451	2160	-75	-397 185
ATOM	940	CA	ALA	134	15.951	21.369	41.451	1.000	14.21
ANISOU	940	CA	ALA	134	1505	1796	2100	116	-570 -33
ATOM	941	C	ALA	134	16.838	21.618	40.246	1.000	15.07
ANISOU	941	C	ALA	134	1766	1511	2450	43	-292 17
ATOM	942	O	ALA	134	17.600	20.750	39.800	1.000	14.36
ANISOU	942	O	ALA	134	1555	1567	2333	-60	-286 52
ATOM	943	CB	ALA	134	14.535	20.925	41.032	1.000	16.97
ANISOU	943	CB	ALA	134	1472	1943	3031	12	-470 -299
ATOM	944	N	ARG	135	16.752	22.808	39.631	1.000	15.48
ANISOU	944	N	ARG	135	1848	1600	2433	14	-341 -2
ATOM	945	CA	ARG	135	17.618	23.153	38.508	1.000	16.07
ANISOU	945	CA	ARG	135	2139	1230	2735	-138	-189 35
ATOM	946	C	ARG	135	19.082	23.057	38.955	1.000	15.70

- 44 -

ANISOU	946	C	ARG	135	2059	1370	2535	-134	27	1	2	1
ATOM	947	O	ARG	135	19.928	22.604	38.176	1.000	18	.	0	7
ANISOU	947	O	ARG	135	2317	2014	2534	108	256	2	7	6
ATOM	948	CB	ARG	135	17.277	24.586	38.096	1.000	21	.	9	6
ANISOU	948	CB	ARG	135	3936	1640	2767	-4	-1480	6	1	4
ATOM	949	CG	ARG	135	17.571	24.989	36.689	1.000	27	.	5	3
ANISOU	949	CG	ARG	135	5112	2482	2866	816	-610	5	9	5
ATOM	950	CD	ARG	135	16.930	26.332	36.393	1.000	23	.	2	7
ANISOU	950	CD	ARG	135	3548	2428	2865	148	61	1	3	7
ATOM	951	NE	ARG	135	15.551	26.309	35.928	1.000	22	.	6	8
ANISOU	951	NE	ARG	135	3488	1575	3556	-116	167	2	9	7
ATOM	952	CZ	ARG	135	14.520	26.858	36.562	1.000	25	.	9	0
ANISOU	952	CZ	ARG	135	3801	2165	3874	921	-506	-1	7	9
ATOM	953	NH1	ARG	135	14.708	27.515	37.702	1.000	23	.	5	0
ANISOU	953	NH1	ARG	135	3582	2378	2969	94	137	5	3	2
ATOM	954	NH2	ARG	135	13.287	26.758	36.035	1.000	24	.	3	0
ANISOU	954	NH2	ARG	135	3520	2441	3272	-101	72	5	8	2
ATOM	955	N	GLU	136	19.403	23.533	40.149	1.000	15	.	7	6
ANISOU	955	N	GLU	136	1897	1696	2396	-178	17	3	1	8
ATOM	956	CA	GLU	136	20.752	23.431	40.694	1.000	15	.	1	6
ANISOU	956	CA	GLU	136	1687	1770	2302	-97	279	1	4	0
ATOM	957	C	GLU	136	21.186	22.001	40.978	1.000	16	.	7	4
ANISOU	957	C	GLU	136	1535	1704	3122	-148	-172	-7	2	
ATOM	958	O	GLU	136	22.350	21.637	40.701	1.000	17	.	4	2
ANISOU	958	O	GLU	136	1710	1908	2999	7	30	9	2	
ATOM	959	CB	GLU	136	20.957	24.284	41.962	1.000	16	.	6	4
ANISOU	959	CB	GLU	136	2048	1785	2487	53	11	-1	6	
ATOM	960	CG	GLU	136	20.762	25.772	41.718	1.000	17	.	8	0
ANISOU	960	CG	GLU	136	2036	1714	3014	-286	-169	1	1	0
ATOM	961	CD	GLU	136	21.534	26.269	40.513	1.000	20	.	9	2
ANISOU	961	CD	GLU	136	2174	2273	3503	-343	70	4	6	9
ATOM	962	OE1	GLU	136	22.742	25.987	40.454	1.000	24	.	9	7
ANISOU	962	OE1	GLU	136	2116	2434	4938	-494	531	2	1	9
ATOM	963	OE2	GLU	136	21.022	27.037	39.672	1.000	24	.	7	7
ANISOU	963	OE2	GLU	136	2975	2618	3817	-708	-133	1	0	2
ATOM	964	N	VAL	137	20.262	21.172	41.450	1.000	15	.	3	4
ANISOU	964	N	VAL	137	1681	1696	2453	-108	-287	1	1	3
ATOM	965	CA	VAL	137	20.568	19.750	41.647	1.000	15	.	9	2
ANISOU	965	CA	VAL	137	1755	1802	2493	83	-4	2	1	0
ATOM	966	C	VAL	137	20.926	19.086	40.326	1.000	15	.	8	6
ANISOU	966	C	VAL	137	1604	1869	2555	-38	-35	6	6	
ATOM	967	O	VAL	137	21.905	18.308	40.174	1.000	16	.	7	0
ANISOU	967	O	VAL	137	1617	2118	2609	72	-151	-9	0	
ATOM	968	CB	VAL	137	19.358	18.990	42.283	1.000	15	.	3	5
ANISOU	968	CB	VAL	137	1729	1663	2440	8	-29	5		
ATOM	969	CG1	VAL	137	19.607	17.478	42.176	1.000	16	.	9	3
ANISOU	969	CG1	VAL	137	1521	1689	3223	160	-345	9	6	
ATOM	970	CG2	VAL	137	19.144	19.420	43.724	1.000	15	.	4	3
ANISOU	970	CG2	VAL	137	1529	2090	2245	-53	-277	1	8	5
ATOM	971	N	LEU	138	20.149	19.407	39.284	1.000	15	.	5	2
ANISOU	971	N	LEU	138	1625	1735	2535	-105	-61	1	0	9
ATOM	972	CA	LEU	138	20.378	18.881	37.936	1.000	15	.	7	4
ANISOU	972	CA	LEU	138	1576	1862	2543	-71	15	5	1	
ATOM	973	C	LEU	138	21.721	19.396	37.406	1.000	17	.	4	2
ANISOU	973	C	LEU	138	1588	2119	2912	-87	162	-4	5	
ATOM	974	O	LEU	138	22.503	18.609	36.846	1.000	19	.	1	3
ANISOU	974	O	LEU	138	1878	2406	2985	186	317	6	2	
ATOM	975	CB	LEU	138	19.211	19.248	36.996	1.000	14	.	7	0
ANISOU	975	CB	LEU	138	1592	1642	2349	-50	141	1	9	0
ATOM	976	CG	LEU	138	17.883	18.541	37.375	1.000	14	.	3	8
ANISOU	976	CG	LEU	138	1657	1409	2399	-44	-4	2	8	8

- 45 -

ATOM 977 CD1 LEU 138 16.774 19.122 36.491 1.000 16.13
 ANISOU 977 CD1 LEU 138 1743 1848 2539 128 -218 1 6 8
 ATOM 978 CD2 LEU 138 17.975 17.027 37.156 1.000 17.48
 ANISOU 978 CD2 LEU 138 2185 1435 3021 -107 -480 2 8 7
 ATOM 979 N ARG 139 21.963 20.708 37.548 1.000 17.44
 ANISOU 979 N ARG 139 1797 2157 2674 -319 238 1 9 2
 ATOM 980 CA ARG 139 23.189 21.319 36.996 1.000 19.06
 ANISOU 980 CA ARG 139 2043 2462 2735 -366 482 3 7 6
 ATOM 981 C ARG 139 24.419 20.734 37.685 1.000 19.72
 ANISOU 981 C ARG 139 1797 2600 3097 -518 482 3 7 6
 ATOM 982 O ARG 139 25.461 20.432 37.094 1.000 20.70
 ANISOU 982 O ARG 139 2046 2469 3350 -288 607 1 9 5
 ATOM 983 CB ARG 139 23.152 22.850 37.101 1.000 24.54
 ANISOU 983 CB ARG 139 2525 2403 4396 -402 951 6 9 0
 ATOM 984 CG ARG 139 23.886 23.665 36.073 1.000 36.05
 ANISOU 984 CG ARG 139 6517 2967 4212 -2176 1609 1 4 0
 ATOM 985 CD ARG 139 23.852 25.148 36.443 1.000 44.95
 ANISOU 985 CD ARG 139 7459 1902 7716 -242 -1324 1 9 3 0
 ATOM 986 NE ARG 139 22.525 25.727 36.547 1.000 43.27
 ANISOU 986 NE ARG 139 6637 3846 5959 -828 -2173 -6 9 8
 ATOM 987 CZ ARG 139 21.821 26.330 35.605 1.000 41.34
 ANISOU 987 CZ ARG 139 5939 4102 5666 497 645 1 1 4 0
 ATOM 988 NH1 ARG 139 22.308 26.436 34.376 1.000 44.01
 ANISOU 988 NH1 ARG 139 6564 4146 6011 550 1393 3 3 6
 ATOM 989 NH2 ARG 139 20.614 26.837 35.833 1.000 45.75
 ANISOU 989 NH2 ARG 139 6162 4618 6602 537 1938 2 4 0 5
 ATOM 990 N ALA 140 24.357 20.566 39.009 1.000 18.77
 ANISOU 990 N ALA 140 1742 2387 3003 -255 145 6 9
 ATOM 991 CA ALA 140 25.532 20.169 39.773 1.000 19.53
 ANISOU 991 CA ALA 140 1583 2641 3197 -28 38 -6 6 8
 ATOM 992 C ALA 140 25.932 18.732 39.490 1.000 18.96
 ANISOU 992 C ALA 140 2018 2342 2843 -67 76 -1 0 3
 ATOM 993 O ALA 140 27.109 18.335 39.626 1.000 21.36
 ANISOU 993 O ALA 140 1900 2436 3778 -2 472 -8 0
 ATOM 994 CB ALA 140 25.273 20.345 41.275 1.000 19.74
 ANISOU 994 CB ALA 140 1824 2592 3084 35 0 -3 6 0
 ATOM 995 N THR 141 24.958 17.943 39.062 1.000 20.32
 ANISOU 995 N THR 141 2014 2209 3498 -115 305 -1 3 8
 ATOM 996 CA THR 141 25.151 16.530 38.717 1.000 17.15
 ANISOU 996 CA THR 141 1870 2039 2609 61 51 2 1 8
 ATOM 997 C THR 141 25.269 16.278 37.208 1.000 17.44
 ANISOU 997 C THR 141 1492 2443 2693 21 278 1 9 9
 ATOM 998 O THR 141 25.343 15.106 36.792 1.000 19.24
 ANISOU 998 O THR 141 1871 2623 2814 63 579 -6 3
 ATOM 999 CB THR 141 24.048 15.629 39.290 1.000 16.79
 ANISOU 999 CB THR 141 1708 2261 2410 83 164 3 1
 ATOM 1000 OG1 THR 141 22.788 16.012 38.710 1.000 17.18
 ANISOU 1000 OG1 THR 141 1894 2235 2399 -101 -53 5 1 8
 ATOM 1001 CG2 THR 141 23.982 15.734 40.807 1.000 17.83
 ANISOU 1001 CG2 THR 141 1521 2878 2377 164 -43 2 0
 ATOM 1002 N GLY 142 25.361 17.301 36.381 1.000 19.69
 ANISOU 1002 N GLY 142 2091 2789 2603 -708 302 2 9 7
 ATOM 1003 CA GLY 142 25.517 17.123 34.923 1.000 19.08
 ANISOU 1003 CA GLY 142 1878 2819 2551 128 -163 2 5 5
 ATOM 1004 C GLY 142 24.284 16.441 34.313 1.000 18.75
 ANISOU 1004 C GLY 142 1972 2410 2744 0 252 -1 1 7
 ATOM 1005 O GLY 142 24.443 15.755 33.315 1.000 22.41
 ANISOU 1005 O GLY 142 2432 2681 3403 -161 571 -6 8 0
 ATOM 1006 N THR 143 23.093 16.650 34.854 1.000 17.28
 ANISOU 1006 N THR 143 1895 2002 2667 67 300 2 4 4
 ATOM 1007 CA THR 143 21.909 15.932 34.393 1.000 16.88

- 46 -

ANISOU	1007	CA	THR	143	1953	2006	2456	164	332	6	6
ATOM	1008	C	THR	143	20.998	16.660	33.432	1.000	17.02		
ANISOU	1008	C	THR	143	2149	1795	2521	82	196	1	1
ATOM	1009	O	THR	143	20.457	17.713	33.764	1.000	20.30		
ANISOU	1009	O	THR	143	2795	1815	3103	344	12	-2	8
ATOM	1010	CB	THR	143	21.085	15.490	35.623	1.000	16.40		
ANISOU	1010	CB	THR	143	1755	2329	2148	-37	95	-4	4
ATOM	1011	OG1	THR	143	21.922	14.692	36.479	1.000	17.82		
ANISOU	1011	OG1	THR	143	2009	2075	2688	-109	39	3	3
ATOM	1012	CG2	THR	143	19.887	14.621	35.270	1.000	19.51		
ANISOU	1012	CG2	THR	143	1957	2290	3167	-192	-94	1	0
ATOM	1013	N	GLU	144	20.742	16.070	32.248	1.000	18.79		
ANISOU	1013	N	GLU	144	2138	2203	2800	47	12	-1	2
ATOM	1014	CA	GLU	144	19.729	16.573	31.334	1.000	20.13		
ANISOU	1014	CA	GLU	144	2202	2696	2750	-292	-41	3	1
ATOM	1015	C	GLU	144	18.637	15.506	31.254	1.000	19.18		
ANISOU	1015	C	GLU	144	2255	2614	2418	-292	230	-1	3
ATOM	1016	O	GLU	144	18.827	14.438	30.665	1.000	21.46		
ANISOU	1016	O	GLU	144	2268	2442	3446	19	649	-8	8
ATOM	1017	CB	AGLU	144	20.250	17.061	30.006	0.753	29.50		
ANISOU	1017	CB	AGLU	144	3376	4266	3566	-855	206	1	5
ATOM	1018	CG	AGLU	144	20.195	18.567	29.741	0.753	36.54		
ANISOU	1018	CG	AGLU	144	6059	3913	3913	-1728	1769	7	9
ATOM	1019	CD	AGLU	144	21.242	19.411	30.426	0.753	33.13		
ANISOU	1019	CD	AGLU	144	4189	3432	4966	104	744	8	8
ATOM	1020	OE1	AGLU	144	21.079	19.690	31.641	0.753	51.91		
ANISOU	1020	OE1	AGLU	144	3684	11101	4940	-868	-202	-5	9
ATOM	1021	OE2	AGLU	144	22.207	19.910	29.807	0.753	50.79		
ANISOU	1021	OE2	AGLU	144	7949	3695	7653	-3071	3099	-1	2
ATOM	1022	CB	BGLU	144	20.372	16.724	29.951	0.247	18.36		
ANISOU	1022	CB	BGLU	144	868	3091	3016	334	16	2	6
ATOM	1023	CG	BGLU	144	21.214	17.988	29.779	0.247	23.54		
ANISOU	1023	CG	BGLU	144	1301	3586	4056	-38	595	5	5
ATOM	1024	CD	BGLU	144	21.150	18.468	28.336	0.247	33.24		
ANISOU	1024	CD	BGLU	144	3589	3975	5064	438	-20	2	3
ATOM	1025	OE1	BGLU	144	20.417	17.818	27.557	0.247	28.68		
ANISOU	1025	OE1	BGLU	144	3222	4813	2861	389	1729	1	2
ATOM	1026	OE2	BGLU	144	21.814	19.464	27.990	0.247	35.35		
ANISOU	1026	OE2	BGLU	144	3176	5148	5108	35	1752	1	5
ATOM	1027	N	PRO	145	17.508	15.724	31.911	1.000	17.11		
ANISOU	1027	N	PRO	145	2132	1825	2543	68	62	1	5
ATOM	1028	CA	PRO	145	16.396	14.781	31.846	1.000	17.41		
ANISOU	1028	CA	PRO	145	2290	1942	2384	-73	400	1	2
ATOM	1029	C	PRO	145	15.966	14.546	30.406	1.000	17.94		
ANISOU	1029	C	PRO	145	2386	1955	2475	-116	292	-1	0
ATOM	1030	O	PRO	145	16.068	15.439	29.557	1.000	18.26		
ANISOU	1030	O	PRO	145	2271	2196	2472	-272	170	4	5
ATOM	1031	CB	PRO	145	15.250	15.493	32.594	1.000	17.07		
ANISOU	1031	CB	PRO	145	2181	1771	2534	35	133	-1	4
ATOM	1032	CG	PRO	145	15.950	16.504	33.464	1.000	17.11		
ANISOU	1032	CG	PRO	145	2341	1841	2319	23	-49	-2	4
ATOM	1033	CD	PRO	145	17.131	16.977	32.649	1.000	17.54		
ANISOU	1033	CD	PRO	145	2178	1601	2884	178	-88	3	0
ATOM	1034	N	ASP	146	15.490	13.346	30.104	1.000	18.15		
ANISOU	1034	N	ASP	146	2140	1965	2790	-60	321	-1	5
ATOM	1035	CA	ASP	146	14.909	13.121	28.775	1.000	18.43		
ANISOU	1035	CA	ASP	146	2487	1664	2853	-329	310	-1	5
ATOM	1036	C	ASP	146	13.809	14.154	28.566	1.000	18.07		
ANISOU	1036	C	ASP	146	2824	1979	2064	-31	208	-3	0
ATOM	1037	O	ASP	146	12.959	14.333	29.422	1.000	18.29		
ANISOU	1037	O	ASP	146	2491	2173	2287	-168	203	-2	3

- 47 -

ATOM	1038	CB	ASP	146	14.221	11.735	28.717	1.000	23.50
ANISOU	1038	CB	ASP	146	3489	1671	3769	-653	908 -665
ATOM	1039	CG	ASP	146	13.636	11.508	27.334	1.000	34.15
ANISOU	1039	CG	ASP	146	4070	4205	4700	-1004	361 -2386
ATOM	1040	OD1	ASP	146	12.393	11.521	27.138	1.000	44.73
ANISOU	1040	OD1	ASP	146	3971	9175	3849	-2156	683 378
ATOM	1041	OD2	ASP	146	14.421	11.229	26.397	1.000	44.78
ANISOU	1041	OD2	ASP	146	4342	8626	4046	-813	289 -2326
ATOM	1042	N	GLY	147	13.901	14.854	27.450	1.000	19.28
ANISOU	1042	N	GLY	147	2622	2331	2374	-635	-72 113
ATOM	1043	CA	GLY	147	12.916	15.878	27.171	1.000	18.58
ANISOU	1043	CA	GLY	147	2463	2607	1991	-550	-234 -36
ATOM	1044	C	GLY	147	13.355	17.262	27.590	1.000	18.25
ANISOU	1044	C	GLY	147	2511	2432	1993	-335	-138 64
ATOM	1045	O	GLY	147	12.586	18.183	27.289	1.000	20.74
ANISOU	1045	O	GLY	147	2469	2739	2673	-182	-144 205
ATOM	1046	N	GLY	148	14.494	17.357	28.286	1.000	17.38
ANISOU	1046	N	GLY	148	2237	2174	2191	-462	-42 -90
ATOM	1047	CA	GLY	148	15.027	18.658	28.672	1.000	16.72
ANISOU	1047	CA	GLY	148	2308	1789	2255	39 -82 -77	
ATOM	1048	C	GLY	148	14.653	19.076	30.085	1.000	13.94
ANISOU	1048	C	GLY	148	1517	1645	2135	77 -201 117	
ATOM	1049	O	GLY	148	13.637	18.634	30.694	1.000	16.29
ANISOU	1049	O	GLY	148	1839	1863	2487	-151	-77 285
ATOM	1050	N	VAL	149	15.431	20.003	30.641	1.000	14.93
ANISOU	1050	N	VAL	149	1624	1780	2269	1 -193 -14	
ATOM	1051	CA	VAL	149	15.275	20.509	32.017	1.000	14.16
ANISOU	1051	CA	VAL	149	1647	1511	2222	92 -195 86	
ATOM	1052	C	VAL	149	13.958	21.218	32.235	1.000	14.37
ANISOU	1052	C	VAL	149	1735	1044	2682	-39	83 188
ATOM	1053	O	VAL	149	13.203	20.970	33.163	1.000	14.63
ANISOU	1053	O	VAL	149	1653	1517	2390	-160	-40 107
ATOM	1054	CB	VAL	149	16.439	21.410	32.417	1.000	14.02
ANISOU	1054	CB	VAL	149	1745	1530	2052	-112	-57 270
ATOM	1055	CG1	VAL	149	16.228	22.101	33.752	1.000	16.48
ANISOU	1055	CG1	VAL	149	2360	1709	2193	-153	-305 87
ATOM	1056	CG2	VAL	149	17.733	20.614	32.482	1.000	17.85
ANISOU	1056	CG2	VAL	149	1618	1937	3226	-59	-52 441
ATOM	1057	N	GLU	150	13.634	22.199	31.371	1.000	15.26
ANISOU	1057	N	GLU	150	1759	1328	2711	186	36 267
ATOM	1058	CA	GLU	150	12.471	23.028	31.687	1.000	14.91
ANISOU	1058	CA	GLU	150	1591	1434	2640	93 13 415	
ATOM	1059	C	GLU	150	11.182	22.237	31.553	1.000	16.66
ANISOU	1059	C	GLU	150	1680	1980	2670	-197	113 199
ATOM	1060	O	GLU	150	10.259	22.408	32.379	1.000	15.89
ANISOU	1060	O	GLU	150	1697	1761	2578	29 79 580	
ATOM	1061	CB	GLU	150	12.531	24.305	30.874	1.000	17.07
ANISOU	1061	CB	GLU	150	1925	1337	3223	254	189 513
ATOM	1062	CG	GLU	150	13.761	25.167	31.220	1.000	19.00
ANISOU	1062	CG	GLU	150	2483	1212	3523	-65	-95 465
ATOM	1063	CD	GLU	150	13.810	25.624	32.658	1.000	20.32
ANISOU	1063	CD	GLU	150	2444	1746	3532	-130	-24 454
ATOM	1064	OE1	GLU	150	12.781	25.749	33.377	1.000	20.88
ANISOU	1064	OE1	GLU	150	2558	1728	3648	29 58 396	
ATOM	1065	OE2	GLU	150	14.913	25.946	33.161	1.000	21.77
ANISOU	1065	OE2	GLU	150	2549	2030	3693	-165	-202 273
ATOM	1066	N	ALA	151	11.050	21.288	30.603	1.000	14.98
ANISOU	1066	N	ALA	151	1649	1710	2334	37 -307 551	
ATOM	1067	CA	ALA	151	9.834	20.475	30.543	1.000	15.79
ANISOU	1067	CA	ALA	151	1820	2045	2136	-173	-198 408
ATOM	1068	C	ALA	151	9.748	19.531	31.724	1.000	15.38

- 48 -

ANISOU	1068	C	ALA	151	1674	1953	2216	165	181	4	4	2	
ATOM	1069	O	ALA	151	8.642	19.186	32.184	1.000	16.51				
ANISOU	1069	O	ALA	151	1778	1852	2643	-152	110	3	3	0	
ATOM	1070	CB	ALA	151	9.823	19.663	29.236	1.000	18.05				
ANISOU	1070	CB	ALA	151	1910	2811	2139	-275	-316	1	6	6	
ATOM	1071	N	PHE	152	10.893	19.135	32.306	1.000	14.25				
ANISOU	1071	N	PHE	152	1858	1132	2423	10	-107	2	6	3	
ATOM	1072	CA	PHE	152	10.893	18.285	33.493	1.000	13.42				
ANISOU	1072	CA	PHE	152	1457	1291	2353	-102	-34	3	0	4	
ATOM	1073	C	PHE	152	10.406	19.056	34.695	1.000	13.93				
ANISOU	1073	C	PHE	152	1481	1400	2412	-43	-165	1	9	6	
ATOM	1074	O	PHE	152	9.679	18.495	35.558	1.000	14.50				
ANISOU	1074	O	PHE	152	1590	1482	2438	-85	25	2	6		
ATOM	1075	CB	PHE	152	12.309	17.744	33.728	1.000	13.95				
ANISOU	1075	CB	PHE	152	1504	1547	2248	-29	111	4	6	3	
ATOM	1076	CG	PHE	152	12.475	16.966	35.011	1.000	14.04				
ANISOU	1076	CG	PHE	152	1747	1386	2200	88	-58	2	4	7	
ATOM	1077	CD1	PHE	152	12.032	15.653	35.076	1.000	13.90				
ANISOU	1077	CD1	PHE	152	1906	1306	2069	165	-36	2	8	1	
ATOM	1078	CD2	PHE	152	13.094	17.499	36.127	1.000	15.67				
ANISOU	1078	CD2	PHE	152	1927	1770	2259	-155	-115	2	3	3	
ATOM	1079	CE1	PHE	152	12.213	14.949	36.263	1.000	14.06				
ANISOU	1079	CE1	PHE	152	1669	1507	2165	182	-282	3	4	7	
ATOM	1080	CE2	PHE	152	13.323	16.799	37.276	1.000	14.83				
ANISOU	1080	CE2	PHE	152	1724	1671	2240	35	-112	1	6	5	
ATOM	1081	CZ	PHE	152	12.861	15.522	37.361	1.000	14.86				
ANISOU	1081	CZ	PHE	152	1994	1734	1916	-162	99	1	1	3	
ATOM	1082	N	LEU	153	10.789	20.324	34.789	1.000	15.25				
ANISOU	1082	N	LEU	153	1742	1355	2696	58	110	1	5	4	
ATOM	1083	CA	LEU	153	10.454	21.151	35.939	1.000	14.65				
ANISOU	1083	CA	LEU	153	1783	1429	2354	-66	16	2	0	3	
ATOM	1084	C	LEU	153	9.082	21.791	35.877	1.000	14.47				
ANISOU	1084	C	LEU	153	1732	1402	2362	-80	76	1	1		
ATOM	1085	O	LEU	153	8.581	22.216	36.953	1.000	15.82				
ANISOU	1085	O	LEU	153	1940	1454	2616	-313	312	-	1	5	7
ATOM	1086	CB	LEU	153	11.537	22.224	36.165	1.000	16.53				
ANISOU	1086	CB	LEU	153	1626	1451	3205	-23	269	-	8	3	
ATOM	1087	CG	LEU	153	12.914	21.685	36.514	1.000	15.90				
ANISOU	1087	CG	LEU	153	1893	2013	2135	-33	-186	-	3	6	
ATOM	1088	CD1	LEU	153	13.922	22.829	36.614	1.000	18.41				
ANISOU	1088	CD1	LEU	153	1732	2473	2791	-156	80	-	8	7	6
ATOM	1089	CD2	LEU	153	12.863	20.883	37.794	1.000	21.76				
ANISOU	1089	CD2	LEU	153	3083	3182	2005	365	261	1	9	3	
ATOM	1090	N	ASP	154	8.473	21.866	34.708	1.000	14.41				
ANISOU	1090	N	ASP	154	1768	1181	2525	-25	-8	2	9	3	
ATOM	1091	CA	ASP	154	7.092	22.373	34.553	1.000	15.90				
ANISOU	1091	CA	ASP	154	1665	1615	2760	-195	27	7	6	9	
ATOM	1092	C	ASP	154	6.216	21.161	34.814	1.000	14.66				
ANISOU	1092	C	ASP	154	1859	1304	2409	-92	143	5	1	5	
ATOM	1093	O	ASP	154	5.995	20.368	33.889	1.000	17.30				
ANISOU	1093	O	ASP	154	2561	1455	2557	-29	314	2	3	4	
ATOM	1094	CB	ASP	154	6.923	22.909	33.125	1.000	18.59				
ANISOU	1094	CB	ASP	154	1905	2077	3081	124	269	1	3	1	7
ATOM	1095	CG	ASP	154	5.461	23.157	32.768	1.000	19.87				
ANISOU	1095	CG	ASP	154	2029	2531	2990	226	129	1	4	3	6
ATOM	1096	OD1	ASP	154	4.561	23.253	33.639	1.000	19.68				
ANISOU	1096	OD1	ASP	154	1949	2209	3318	92	221	4	9	6	
ATOM	1097	OD2	ASP	154	5.207	23.189	31.554	1.000	23.73				
ANISOU	1097	OD2	ASP	154	2512	3475	3029	246	-137	6	5	3	
ATOM	1098	N	CYS	155	5.831	20.904	36.070	1.000	14.25				
ANISOU	1098	N	CYS	155	1708	1365	2342	-101	-62	5	4	6	

- 49 -

ATOM	1099	CA	CYS	155	5.418	19.569	36.468	1.000	13.45
ANISOU	1099	CA	CYS	155	1608	1346	2158	-191	4 4 5 8
ATOM	1100	C	CYS	155	4.157	19.574	37.302	1.000	12.49
ANISOU	1100	C	CYS	155	1644	1331	1772	-200	-148 6 2
ATOM	1101	O	CYS	155	3.224	20.303	36.941	1.000	14.55
ANISOU	1101	O	CYS	155	1633	1492	2402	-122	-111 4 4 2
ATOM	1102	CB	CYS	155	6.664	18.872	37.098	1.000	14.37
ANISOU	1102	CB	CYS	155	1907	1366	2186	122	-137 2 1 1
ATOM	1103	SG	CYS	155	7.265	19.595	38.641	1.000	14.99
ANISOU	1103	SG	CYS	155	1561	1821	2315	-74	-98 1 8 2
ATOM	1104	N	GLU	156	4.060	18.706	38.316	1.000	12.89
ANISOU	1104	N	GLU	156	1575	1379	1945	-130	29 1 9 4
ATOM	1105	CA	GLU	156	2.788	18.447	39.029	1.000	12.98
ANISOU	1105	CA	GLU	156	1508	1311	2114	-210	21 1 4 0
ATOM	1106	C	GLU	156	2.987	18.676	40.510	1.000	12.34
ANISOU	1106	C	GLU	156	1414	1198	2078	102	24 2 0 4
ATOM	1107	O	GLU	156	2.828	17.757	41.289	1.000	14.89
ANISOU	1107	O	GLU	156	1875	1425	2359	-15	-54 4 4 2
ATOM	1108	CB	GLU	156	2.278	17.047	38.678	1.000	14.48
ANISOU	1108	CB	GLU	156	1968	1323	2213	-279	120 8 7
ATOM	1109	CG	GLU	156	1.855	17.038	37.227	1.000	14.86
ANISOU	1109	CG	GLU	156	1894	1526	2227	-120	95 -15 2
ATOM	1110	CD	GLU	156	0.523	17.687	36.932	1.000	17.10
ANISOU	1110	CD	GLU	156	2091	1976	2431	44 -4	1 4 4
ATOM	1111	OE1	GLU	156	-0.204	17.967	37.886	1.000	17.98
ANISOU	1111	OE1	GLU	156	1811	2155	2866	-35	10 -35 5
ATOM	1112	OE2	GLU	156	0.214	17.990	35.759	1.000	20.99
ANISOU	1112	OE2	GLU	156	2854	2419	2704	-386	-516 5 6 2
ATOM	1113	N	PRO	157	3.292	19.893	40.958	1.000	12.09
ANISOU	1113	N	PRO	157	1314	1347	1934	12 -48	2 4 9
ATOM	1114	CA	PRO	157	3.576	20.121	42.391	1.000	13.28
ANISOU	1114	CA	PRO	157	1425	1696	1924	-68	117 1 4 7
ATOM	1115	C	PRO	157	2.330	19.996	43.248	1.000	12.87
ANISOU	1115	C	PRO	157	1236	1737	1916	-214	-47 1 2 4
ATOM	1116	O	PRO	157	1.192	20.190	42.744	1.000	13.73
ANISOU	1116	O	PRO	157	1286	1717	2214	-190	-17 1 4 3
ATOM	1117	CB	PRO	157	4.061	21.580	42.407	1.000	13.94
ANISOU	1117	CB	PRO	157	1518	1729	2047	-289	-166 2 4 7
ATOM	1118	CG	PRO	157	3.363	22.184	41.226	1.000	13.06
ANISOU	1118	CG	PRO	157	1558	1518	1887	-32	-158 -8 8
ATOM	1119	CD	PRO	157	3.494	21.128	40.167	1.000	12.03
ANISOU	1119	CD	PRO	157	1521	1081	1968	-2 -7	1 2 1
ATOM	1120	N	LEU	158	2.542	19.738	44.526	1.000	13.02
ANISOU	1120	N	LEU	158	1554	1493	1899	-124	148 7 3
ATOM	1121	CA	LEU	158	1.438	19.699	45.496	1.000	12.72
ANISOU	1121	CA	LEU	158	1465	1552	1815	-126	-14 3 6
ATOM	1122	C	LEU	158	1.927	20.389	46.772	1.000	12.90
ANISOU	1122	C	LEU	158	1230	1715	1957	-27	-29 -8 0
ATOM	1123	O	LEU	158	2.975	19.977	47.289	1.000	14.06
ANISOU	1123	O	LEU	158	1374	1666	2304	59 -257	-23 6
ATOM	1124	CB	LEU	158	1.046	18.244	45.815	1.000	13.58
ANISOU	1124	CB	LEU	158	1673	1590	1896	-213	57 1 7 1
ATOM	1125	CG	LEU	158	0.044	18.030	46.945	1.000	14.84
ANISOU	1125	CG	LEU	158	1471	1774	2396	-16	262 2 4 2
ATOM	1126	CD1	LEU	158	-1.333	18.635	46.671	1.000	16.96
ANISOU	1126	CD1	LEU	158	1485	2196	2764	5 -148	-4 0 1
ATOM	1127	CD2	LEU	158	-0.142	16.539	47.161	1.000	14.98
ANISOU	1127	CD2	LEU	158	1976	1820	1897	-390	171 7 9
ATOM	1128	N	LEU	159	1.139	21.306	47.283	1.000	13.44
ANISOU	1128	N	LEU	159	1509	1434	2165	43 -87	-11 9
ATOM	1129	CA	LEU	159	1.443	21.963	48.571	1.000	13.39

- 50 -

ANISOU	1129	CA	LEU	159	1438	1555	2095	-36	-80	-9	1
ATOM	1130	C	LEU	159	0.419	21.494	49.602	1.000	14.49		
ANISOU	1130	C	LEU	159	1336	2034	2135	-152	-208	-3	8
ATOM	1131	O	LEU	159	-0.790	21.596	49.419	1.000	15.09		
ANISOU	1131	O	LEU	159	1414	1999	2319	90	-131	9	0
ATOM	1132	CB	LEU	159	1.390	23.466	48.394	1.000	15.28		
ANISOU	1132	CB	LEU	159	1720	1447	2639	55	-325	-19	7
ATOM	1133	CG	LEU	159	1.484	24.320	49.669	1.000	17.11		
ANISOU	1133	CG	LEU	159	2146	1689	2665	363	-332	-34	3
ATOM	1134	CD1	LEU	159	2.775	24.114	50.453	1.000	18.70		
ANISOU	1134	CD1	LEU	159	2276	1759	3070	379	-687	-54	0
ATOM	1135	CD2	LEU	159	1.312	25.801	49.291	1.000	21.00		
ANISOU	1135	CD2	LEU	159	2918	1535	3526	439	-692	-38	2
ATOM	1136	N	ARG	160	0.916	21.107	50.774	1.000	14.37		
ANISOU	1136	N	ARG	160	1688	1709	2063	-101	-186	4	7
ATOM	1137	CA	ARG	160	0.055	20.747	51.901	1.000	15.61		
ANISOU	1137	CA	ARG	160	1726	1990	2217	-64	90	-11	8
ATOM	1138	C	ARG	160	0.480	21.501	53.155	1.000	15.40		
ANISOU	1138	C	ARG	160	1557	2158	2135	-34	-46	-3	8
ATOM	1139	O	ARG	160	1.639	21.401	53.576	1.000	16.32		
ANISOU	1139	O	ARG	160	1528	2508	2164	63	41	-10	4
ATOM	1140	CB	ARG	160	0.048	19.263	52.227	1.000	16.13		
ANISOU	1140	CB	ARG	160	2134	2084	1912	-127	-30	12	9
ATOM	1141	CG	ARG	160	-0.594	18.410	51.155	1.000	17.17		
ANISOU	1141	CG	ARG	160	1963	1934	2628	-140	-212	-6	0
ATOM	1142	CD	ARG	160	-0.672	16.959	51.627	1.000	18.16		
ANISOU	1142	CD	ARG	160	2767	1965	2166	125	-330	-3	5
ATOM	1143	NE	ARG	160	-1.382	16.102	50.682	1.000	18.11		
ANISOU	1143	NE	ARG	160	2408	1775	2699	-56	-308	2	0
ATOM	1144	CZ	ARG	160	-1.221	14.789	50.581	1.000	16.76		
ANISOU	1144	CZ	ARG	160	2191	1748	2428	-97	55	17	4
ATOM	1145	NH1	ARG	160	-0.326	14.192	51.374	1.000	20.55		
ANISOU	1145	NH1	ARG	160	2306	2012	3491	-26	-457	3	0
ATOM	1146	NH2	ARG	160	-1.908	14.095	49.689	1.000	19.23		
ANISOU	1146	NH2	ARG	160	2502	2031	2774	181	-147	-33	8
ATOM	1147	N	PHE	161	-0.469	22.257	53.755	1.000	15.36		
ANISOU	1147	N	PHE	161	1604	2120	2111	-37	-63	-12	8
ATOM	1148	CA	PHE	161	-0.209	22.975	54.999	1.000	16.25		
ANISOU	1148	CA	PHE	161	2173	1774	2227	-71	-187	-8	9
ATOM	1149	C	PHE	161	-1.030	22.236	56.069	1.000	16.98		
ANISOU	1149	C	PHE	161	1980	2432	2041	-217	-161	-16	2
ATOM	1150	O	PHE	161	-2.248	22.113	55.948	1.000	20.38		
ANISOU	1150	O	PHE	161	1981	3291	2473	-190	-191	-7	2
ATOM	1151	CB	PHE	161	-0.683	24.431	54.862	1.000	19.76		
ANISOU	1151	CB	PHE	161	2065	1903	3540	167	355	-19	8
ATOM	1152	CG	PHE	161	-0.379	25.259	56.109	1.000	23.61		
ANISOU	1152	CG	PHE	161	3026	1905	4041	836	-59	-59	1
ATOM	1153	CD1	PHE	161	-1.194	25.304	57.228	1.000	28.25		
ANISOU	1153	CD1	PHE	161	3992	2474	4268	1077	369	-12	5
ATOM	1154	CD2	PHE	161	0.807	25.978	56.141	1.000	26.62		
ANISOU	1154	CD2	PHE	161	4015	2483	3616	-130	-927	-10	6
ATOM	1155	CE1	PHE	161	-0.850	25.992	58.383	1.000	35.29		
ANISOU	1155	CE1	PHE	161	6873	2097	4437	1538	-135	-13	9
ATOM	1156	CE2	PHE	161	1.153	26.723	57.258	1.000	33.63		
ANISOU	1156	CE2	PHE	161	4643	3240	4894	1263	-2085	-12	6
ATOM	1157	CZ	PHE	161	0.320	26.726	58.363	1.000	36.44		
ANISOU	1157	CZ	PHE	161	6071	4282	3493	1455	-2477	-10	4
ATOM	1158	N	ARG	162	-0.358	21.767	57.130	1.000	17.59		
ANISOU	1158	N	ARG	162	2095	2487	2103	-118	-135	-6	9
ATOM	1159	CA	ARG	162	-1.072	21.078	58.199	1.000	18.27		
ANISOU	1159	CA	ARG	162	2769	2414	1758	6	178	-3	7

- 51 -

ATOM 1160 C ARG 162 -0.880 21.758 59.553 1.000 20.16
 ANISOU 1160 C ARG 162 2110 3341 2210 -36 41 -960
 ATOM 1161 O ARG 162 0.217 22.160 59.893 1.000 19.61
 ANISOU 1161 O ARG 162 2257 2993 2201 -194 -73 -359
 ATOM 1162 CB ARG 162 -0.580 19.640 58.356 1.000 20.81
 ANISOU 1162 CB ARG 162 2958 2275 2675 -129 6 -169
 ATOM 1163 CG ARG 162 -0.843 18.724 57.166 1.000 19.90
 ANISOU 1163 CG ARG 162 3044 2073 2443 -112 254 -38
 ATOM 1164 CD ARG 162 -0.182 17.383 57.393 1.000 28.02
 ANISOU 1164 CD ARG 162 5599 2038 3010 381 -14 114
 ATOM 1165 NE ARG 162 -0.369 16.420 56.326 1.000 27.74
 ANISOU 1165 NE ARG 162 4151 2294 4097 555 -687 -434
 ATOM 1166 CZ ARG 162 -1.278 15.445 56.370 1.000 31.11
 ANISOU 1166 CZ ARG 162 2560 3729 5531 470 -350 -1152
 ATOM 1167 NH1 ARG 162 -2.092 15.324 57.403 1.000 42.97
 ANISOU 1167 NH1 ARG 162 3475 5906 6946 -579 1019 -2492
 ATOM 1168 NH2 ARG 162 -1.329 14.603 55.353 1.000 29.64
 ANISOU 1168 NH2 ARG 162 3066 2738 5458 120 -143 -708
 ATOM 1169 N TYR 163 -1.956 21.780 60.311 1.000 19.52
 ANISOU 1169 N TYR 163 2394 2901 2120 147 263 -763
 ATOM 1170 CA TYR 163 -1.943 22.102 61.732 1.000 22.74
 ANISOU 1170 CA TYR 163 3312 3107 2219 369 302 -878
 ATOM 1171 C TYR 163 -2.037 20.800 62.536 1.000 24.20
 ANISOU 1171 C TYR 163 2802 3901 2492 -222 253 -189
 ATOM 1172 O TYR 163 -2.992 20.049 62.274 1.000 28.02
 ANISOU 1172 O TYR 163 2305 4409 3934 -202 -126 399
 ATOM 1173 CB TYR 163 -3.198 22.912 62.114 1.000 28.98
 ANISOU 1173 CB TYR 163 3861 3231 3920 267 1196 -1783
 ATOM 1174 CG TYR 163 -3.342 22.997 63.623 1.000 25.58
 ANISOU 1174 CG TYR 163 2572 3382 3767 543 749 -1204
 ATOM 1175 CD1 TYR 163 -2.458 23.826 64.319 1.000 37.32
 ANISOU 1175 CD1 TYR 163 3654 6112 4413 -759 884 -2373
 ATOM 1176 CD2 TYR 163 -4.315 22.333 64.345 1.000 29.13
 ANISOU 1176 CD2 TYR 163 2622 3994 4452 749 1084 -769
 ATOM 1177 CE1 TYR 163 -2.546 23.966 65.702 1.000 38.28
 ANISOU 1177 CE1 TYR 163 2905 7138 4503 -454 987 -2740
 ATOM 1178 CE2 TYR 163 -4.396 22.431 65.726 1.000 37.36
 ANISOU 1178 CE2 TYR 163 3220 6336 4640 -273 1997 -1618
 ATOM 1179 CZ TYR 163 -3.500 23.250 66.393 1.000 49.85
 ANISOU 1179 CZ TYR 163 5272 8795 4872 -1810 1593 -2223
 ATOM 1180 OH TYR 163 -3.595 23.365 67.768 1.000 44.81
 ANISOU 1180 OH TYR 163 5246 7368 4413 -222 270 -496
 ATOM 1181 N PHE 164 -1.098 20.651 63.448 1.000 24.84
 ANISOU 1181 N PHE 164 2905 3368 3164 -89 -125 -361
 ATOM 1182 CA PHE 164 -1.045 19.532 64.370 1.000 28.14
 ANISOU 1182 CA PHE 164 3538 3957 3195 223 -163 -30
 ATOM 1183 C PHE 164 -1.360 20.003 65.787 1.000 26.67
 ANISOU 1183 C PHE 164 2964 3937 3234 -473 -194 -257
 ATOM 1184 O PHE 164 -0.540 20.730 66.342 1.000 31.26
 ANISOU 1184 O PHE 164 3119 4888 3869 -959 -260 -519
 ATOM 1185 CB PHE 164 0.347 18.881 64.396 1.000 27.86
 ANISOU 1185 CB PHE 164 3423 3725 3436 76 -199 -32
 ATOM 1186 CG PHE 164 0.744 18.301 63.052 1.000 26.77
 ANISOU 1186 CG PHE 164 2914 3474 3785 -598 74 -275
 ATOM 1187 CD1 PHE 164 1.435 19.093 62.143 1.000 26.16
 ANISOU 1187 CD1 PHE 164 2827 3836 3278 135 -615 711
 ATOM 1188 CD2 PHE 164 0.414 16.996 62.717 1.000 31.24
 ANISOU 1188 CD2 PHE 164 4365 2808 4698 349 -298 -96
 ATOM 1189 CE1 PHE 164 1.787 18.609 60.894 1.000 30.09
 ANISOU 1189 CE1 PHE 164 3609 5052 2771 -148 -1030 641
 ATOM 1190 CE2 PHE 164 0.786 16.501 61.475 1.000 38.25

- 52 -

ANISOU	1190	CE2	PHE	164	6659	4077	3797	-740	-1363	-612
ATOM	1191	CZ	PHE	164	1.494	17.298	60.588	1.000	32.74	
ANISOU	1191	CZ	PHE	164	3189	5078	4172	712	-944	-385
ATOM	1192	N	PRO	165	-2.469	19.609	66.379	1.000	30.62	
ANISOU	1192	N	PRO	165	3876	4009	3751	-1371	344	-508
ATOM	1193	CA	PRO	165	-2.670	19.813	67.809	1.000	33.09	
ANISOU	1193	CA	PRO	165	3299	5764	3510	-190	80	236
ATOM	1194	C	PRO	165	-1.459	19.408	68.638	1.000	36.32	
ANISOU	1194	C	PRO	165	3538	5745	4518	664	-191	-234
ATOM	1195	O	PRO	165	-0.776	18.428	68.371	1.000	32.94	
ANISOU	1195	O	PRO	165	4268	4761	3487	220	501	387
ATOM	1196	CB	PRO	165	-3.882	18.929	68.123	1.000	38.44	
ANISOU	1196	CB	PRO	165	3807	6924	3873	-765	271	827
ATOM	1197	CG	PRO	165	-4.635	18.842	66.845	1.000	35.82	
ANISOU	1197	CG	PRO	165	2595	7020	3995	5	688	-828
ATOM	1198	CD	PRO	165	-3.690	19.130	65.710	1.000	33.90	
ANISOU	1198	CD	PRO	165	3192	5919	3770	-1149	194	169
ATOM	1199	N	LEU	178	7.727	7.453	68.180	1.000	64.52	
ANISOU	1199	N	LEU	178	12297	5376	6843	278	-218	3721
ATOM	1200	CA	LEU	178	7.629	8.260	66.973	1.000	43.31	
ANISOU	1200	CA	LEU	178	10557	2730	3168	-984	-2821	-135
ATOM	1201	C	LEU	178	6.159	8.539	66.662	1.000	47.36	
ANISOU	1201	C	LEU	178	9239	3530	5225	-2598	-1186	1204
ATOM	1202	O	LEU	178	5.314	7.659	66.796	1.000	56.53	
ANISOU	1202	O	LEU	178	11777	5626	4076	-4835	1265	-602
ATOM	1203	CB	LEU	178	8.222	7.582	65.746	1.000	55.55	
ANISOU	1203	CB	LEU	178	11470	3734	5902	-1314	-1197	-1822
ATOM	1204	CG	LEU	178	9.662	7.092	65.774	1.000	62.34	
ANISOU	1204	CG	LEU	178	10812	5116	7760	-1971	194	-443
ATOM	1205	CD1	LEU	178	9.916	6.185	64.579	1.000	54.23	
ANISOU	1205	CD1	LEU	178	9626	4989	5988	1878	-3799	511
ATOM	1206	CD2	LEU	178	10.633	8.264	65.773	1.000	66.44	
ANISOU	1206	CD2	LEU	178	11265	3454	10526	-1170	4090	-516
ATOM	1207	N	ARG	179	5.879	9.751	66.192	1.000	52.90	
ANISOU	1207	N	ARG	179	7853	3826	8421	102	1230	1031
ATOM	1208	CA	ARG	179	4.495	10.033	65.807	1.000	51.26	
ANISOU	1208	CA	ARG	179	7235	4820	7421	-229	1890	-383
ATOM	1209	C	ARG	179	4.242	9.563	64.383	1.000	55.25	
ANISOU	1209	C	ARG	179	7178	6083	7731	-946	2260	-1134
ATOM	1210	O	ARG	179	3.120	9.211	64.021	1.000	58.51	
ANISOU	1210	O	ARG	179	7036	7628	7565	-1820	3675	-2851
ATOM	1211	CB	ARG	179	4.180	11.512	66.040	1.000	41.49	
ANISOU	1211	CB	ARG	179	6600	4448	4716	-155	1916	1137
ATOM	1212	CG	ARG	179	3.293	11.700	67.277	1.000	43.15	
ANISOU	1212	CG	ARG	179	6120	5908	4367	90	1338	530
ATOM	1213	CD	ARG	179	1.888	12.059	66.833	1.000	47.63	
ANISOU	1213	CD	ARG	179	6180	7453	4463	195	860	-531
ATOM	1214	NE	ARG	179	1.459	13.367	67.269	1.000	52.00	
ANISOU	1214	NE	ARG	179	7384	7834	4539	1669	-1168	-538
ATOM	1215	CZ	ARG	179	1.322	14.470	66.556	1.000	64.81	
ANISOU	1215	CZ	ARG	179	10838	8000	5788	1457	-1107	63
ATOM	1216	NH1	ARG	179	1.637	14.518	65.268	1.000	59.74	
ANISOU	1216	NH1	ARG	179	9535	8090	5074	3628	-2691	445
ATOM	1217	NH2	ARG	179	0.907	15.606	67.117	1.000	65.83	
ANISOU	1217	NH2	ARG	179	10451	9083	5478	4171	-776	1200
ATOM	1218	N	MET	180	5.304	9.501	63.589	1.000	43.96	
ANISOU	1218	N	MET	180	5383	3769	7550	705	852	-1245
ATOM	1219	CA	MET	180	5.264	9.035	62.210	1.000	40.44	
ANISOU	1219	CA	MET	180	2356	5467	7543	-398	574	-1482
ATOM	1220	C	MET	180	6.552	8.258	61.920	1.000	43.91	
ANISOU	1220	C	MET	180	2731	6220	7733	18	320	-2324

- 53 -

ATOM	1221	O	MET	180	7.629	8.679	62.327	1.000	39.46
ANISOU	1221	O	MET	180	2377	5064	7554	-395	906 -912
ATOM	1222	CB	MET	180	5.129	10.189	61.219	1.000	49.84
ANISOU	1222	CB	MET	180	2749	7966	8223	-452	-1114 7 2
ATOM	1223	CG	MET	180	5.339	9.818	59.757	1.000	62.58
ANISOU	1223	CG	MET	180	7280	8911	7587	-2331	-3353 -505
ATOM	1224	SD	MET	180	4.622	11.015	58.608	1.000	74.24
ANISOU	1224	SD	MET	180	7480	13510	7216	4918	-262 -905
ATOM	1225	CE	MET	180	4.501	10.037	57.110	1.000	79.59
ANISOU	1225	CE	MET	180	6119	20000	4120	-1978	1874 -912
ATOM	1226	N	ALA	181	6.376	7.112	61.275	1.000	37.44
ANISOU	1226	N	ALA	181	3523	5646	5055	-271	882 -1132
ATOM	1227	CA	ALA	181	7.407	6.140	60.986	1.000	37.40
ANISOU	1227	CA	ALA	181	3980	3980	6250	-625	2048 4 6 1
ATOM	1228	C	ALA	181	8.287	6.591	59.837	1.000	31.49
ANISOU	1228	C	ALA	181	2975	3842	5149	-32	920 9 5 6
ATOM	1229	O	ALA	181	7.834	7.393	58.997	1.000	30.77
ANISOU	1229	O	ALA	181	2903	4021	4765	197	-98 1 6 4
ATOM	1230	CB	ALA	181	6.727	4.817	60.620	1.000	42.66
ANISOU	1230	CB	ALA	181	4105	4284	7820	-1023	1629 5 5 7
ATOM	1231	N	PRO	182	9.541	6.137	59.840	1.000	24.52
ANISOU	1231	N	PRO	182	2782	4237	2296	-240	-76 3 2 0
ATOM	1232	CA	PRO	182	10.442	6.667	58.820	1.000	20.55
ANISOU	1232	CA	PRO	182	2612	2870	2326	-335	-117 -6 5
ATOM	1233	C	PRO	182	9.958	6.402	57.408	1.000	19.31
ANISOU	1233	C	PRO	182	2609	2491	2236	-391	48 -8 6
ATOM	1234	O	PRO	182	9.448	5.326	57.080	1.000	21.68
ANISOU	1234	O	PRO	182	2991	2486	2759	-440	-340 -5 5
ATOM	1235	CB	PRO	182	11.768	5.939	59.047	1.000	24.98
ANISOU	1235	CB	PRO	182	2589	3860	3042	-170	-286 1 5 3
ATOM	1236	CG	PRO	182	11.681	5.351	60.393	1.000	28.42
ANISOU	1236	CG	PRO	182	3352	3582	3863	656	321 1 0 3 8
ATOM	1237	CD	PRO	182	10.215	5.210	60.747	1.000	32.21
ANISOU	1237	CD	PRO	182	3333	4905	4000	-826	-390 1 7 8 5
ATOM	1238	N	HIS	183	10.111	7.414	56.561	1.000	19.27
ANISOU	1238	N	HIS	183	2131	2658	2533	-274	-204 1 7 6
ATOM	1239	CA	HIS	183	9.757	7.306	55.144	1.000	18.01
ANISOU	1239	CA	HIS	183	1882	2311	2652	-341	-455 3 4 6
ATOM	1240	C	HIS	183	10.749	8.124	54.337	1.000	15.74
ANISOU	1240	C	HIS	183	1964	1560	2456	-75	-352 1 2 8
ATOM	1241	O	HIS	183	11.355	9.061	54.868	1.000	18.14
ANISOU	1241	O	HIS	183	2297	2093	2504	-509	-127 -1 3 5
ATOM	1242	CB	HIS	183	8.338	7.781	54.835	1.000	18.66
ANISOU	1242	CB	HIS	183	1970	2173	2945	-136	-243 3 7 1
ATOM	1243	CG	HIS	183	8.089	9.120	55.447	1.000	26.67
ANISOU	1243	CG	HIS	183	3100	2751	4281	262	222 -3 0 6
ATOM	1244	ND1	HIS	183	7.884	9.362	56.800	1.000	35.36
ANISOU	1244	ND1	HIS	183	4432	4078	4926	-1190	1466 -1 4 5 4
ATOM	1245	CD2	HIS	183	8.051	10.311	54.821	1.000	33.00
ANISOU	1245	CD2	HIS	183	4117	2522	5898	1687	-677 -1 7 3
ATOM	1246	CE1	HIS	183	7.739	10.658	56.980	1.000	35.91
ANISOU	1246	CE1	HIS	183	2611	4468	6565	-472	-625 -2 6 1 6
ATOM	1247	NE2	HIS	183	7.829	11.251	55.798	1.000	40.55
ANISOU	1247	NE2	HIS	183	4375	3417	7614	1821	-1013 -1 5 9 0
ATOM	1248	N	TYR	184	10.890	7.778	53.061	1.000	15.68
ANISOU	1248	N	TYR	184	1973	1551	2434	-124	-470 1 0 7
ATOM	1249	CA	TYR	184	11.605	8.685	52.152	1.000	14.81
ANISOU	1249	CA	TYR	184	1798	1392	2438	147	-312 1 4 5
ATOM	1250	C	TYR	184	10.572	9.239	51.169	1.000	14.53
ANISOU	1250	C	TYR	184	1656	1449	2416	-70	-399 9 8
ATOM	1251	O	TYR	184	9.468	8.728	51.045	1.000	15.83

- 54 -

ANISOU	1251	O	TYR	184	1717	1383	2916	-103	-443	1	5	0
ATOM	1252	CB	TYR	184	12.699	8.004	51.360	1.000	15.66			
ANISOU	1252	CB	TYR	184	1686	1323	2943	69	-366	-1	6	8
ATOM	1253	CG	TYR	184	12.383	6.785	50.562	1.000	14.85			
ANISOU	1253	CG	TYR	184	1743	1313	2586	109	-567	4	3	
ATOM	1254	CD1	TYR	184	12.200	5.540	51.185	1.000	15.49			
ANISOU	1254	CD1	TYR	184	1549	1315	3021	-29	-575	1	9	0
ATOM	1255	CD2	TYR	184	12.329	6.836	49.165	1.000	15.89			
ANISOU	1255	CD2	TYR	184	1724	1763	2552	55	-27	-6	4	
ATOM	1256	CE1	TYR	184	11.962	4.396	50.442	1.000	15.61			
ANISOU	1256	CE1	TYR	184	1695	1244	2992	229	-137	1	1	3
ATOM	1257	CE2	TYR	184	12.130	5.661	48.447	1.000	17.52			
ANISOU	1257	CE2	TYR	184	2340	1776	2540	4	83	-9	0	
ATOM	1258	CZ	TYR	184	11.915	4.449	49.083	1.000	16.96			
ANISOU	1258	CZ	TYR	184	1695	1736	3014	-156	-480	3	4	
ATOM	1259	OH	TYR	184	11.682	3.325	48.310	1.000	18.81			
ANISOU	1259	OH	TYR	184	2020	1775	3352	260	-277	-3	1	2
ATOM	1260	N	ASP	185	10.924	10.330	50.502	1.000	14.36			
ANISOU	1260	N	ASP	185	1518	1599	2338	87	-225	2	7	6
ATOM	1261	CA	ASP	185	10.026	11.005	49.574	1.000	13.88			
ANISOU	1261	CA	ASP	185	1875	1322	2078	141	-364	-4	2	
ATOM	1262	C	ASP	185	10.240	10.490	48.152	1.000	12.57			
ANISOU	1262	C	ASP	185	1182	1385	2211	-160	-77	-1	3	0
ATOM	1263	O	ASP	185	11.357	10.135	47.824	1.000	14.14			
ANISOU	1263	O	ASP	185	1177	1637	2559	-135	146	1	4	0
ATOM	1264	CB	ASP	185	10.294	12.521	49.580	1.000	14.97			
ANISOU	1264	CB	ASP	185	1879	1293	2517	121	-186	-1	5	9
ATOM	1265	CG	ASP	185	9.702	13.155	50.830	1.000	17.61			
ANISOU	1265	CG	ASP	185	2680	1659	2351	232	-13	-1	7	2
ATOM	1266	OD1	ASP	185	9.507	12.466	51.856	1.000	23.69			
ANISOU	1266	OD1	ASP	185	3553	3133	2314	443	-302	5	2	1
ATOM	1267	OD2	ASP	185	9.174	14.257	50.742	1.000	24.32			
ANISOU	1267	OD2	ASP	185	4063	1730	3449	644	1140	-1	6	
ATOM	1268	N	LEU	186	9.141	10.465	47.382	1.000	12.57			
ANISOU	1268	N	LEU	186	1271	1378	2126	-117	-117	-1	1	7
ATOM	1269	CA	LEU	186	9.169	10.091	45.986	1.000	12.92			
ANISOU	1269	CA	LEU	186	1533	1225	2150	-331	-84	-1	7	5
ATOM	1270	C	LEU	186	9.134	11.292	45.052	1.000	14.12			
ANISOU	1270	C	LEU	186	1730	1307	2330	-93	-165	5	5	
ATOM	1271	O	LEU	186	8.971	11.173	43.849	1.000	20.12			
ANISOU	1271	O	LEU	186	3721	1643	2280	-423	99	9	2	
ATOM	1272	CB	LEU	186	8.040	9.106	45.609	1.000	13.72			
ANISOU	1272	CB	LEU	186	1509	1310	2393	-270	-375	-	6	
ATOM	1273	CG	LEU	186	8.020	7.811	46.438	1.000	15.92			
ANISOU	1273	CG	LEU	186	1549	1141	3361	-145	-307	1	6	8
ATOM	1274	CD1	LEU	186	6.929	6.908	45.866	1.000	19.36			
ANISOU	1274	CD1	LEU	186	1686	1845	3825	-700	-209	3	9	6
ATOM	1275	CD2	LEU	186	9.369	7.115	46.341	1.000	18.32			
ANISOU	1275	CD2	LEU	186	1689	1742	3528	200	-432	1	7	9
ATOM	1276	N	SER	187	9.286	12.494	45.618	1.000	13.60			
ANISOU	1276	N	SER	187	1326	1234	2608	-26	-95	1	3	7
ATOM	1277	CA	SER	187	9.388	13.734	44.826	1.000	13.22			
ANISOU	1277	CA	SER	187	1489	1197	2338	-54	-68	2	9	
ATOM	1278	C	SER	187	10.736	13.853	44.134	1.000	12.79			
ANISOU	1278	C	SER	187	1482	1186	2192	-17	-114	-	9	0
ATOM	1279	O	SER	187	11.683	13.076	44.356	1.000	14.50			
ANISOU	1279	O	SER	187	1532	1257	2720	76	-224	-1	1	3
ATOM	1280	CB	SER	187	9.201	14.915	45.811	1.000	12.87			
ANISOU	1280	CB	SER	187	1463	1282	2147	164	-154	9	8	
ATOM	1281	OG	SER	187	10.296	14.873	46.716	1.000	13.22			
ANISOU	1281	OG	SER	187	1589	1420	2015	-34	-143	2	2	4

- 55 -

ATOM 1282 N MET 188 10.898 14.844 43.292 1.000 13.44
 ANISOU 1282 N MET 188 1552 1334 2221 -64 -34 -2 6
 ATOM 1283 CA MET 188 12.215 15.380 42.878 1.000 12.11
 ANISOU 1283 CA MET 188 1508 1261 1833 29 -60 -6 1
 ATOM 1284 C MET 188 12.853 16.022 44.104 1.000 12.78
 ANISOU 1284 C MET 188 1563 1156 2136 167 -311 -4 2
 ATOM 1285 O MET 188 13.896 15.550 44.600 1.000 13.40
 ANISOU 1285 O MET 188 1408 1390 2294 116 -264 -2 6
 ATOM 1286 CB MET 188 12.038 16.300 41.667 1.000 13.66
 ANISOU 1286 CB MET 188 1565 1501 2123 44 -161 2 0 7
 ATOM 1287 CG MET 188 13.296 17.095 41.315 1.000 14.05
 ANISOU 1287 CG MET 188 1697 1595 2046 66 150 1 3 3
 ATOM 1288 SD MET 188 14.600 15.971 40.752 1.000 14.96
 ANISOU 1288 SD MET 188 1565 1591 2529 109 -81 1 1 0
 ATOM 1289 CE MET 188 16.005 17.102 40.686 1.000 17.74
 ANISOU 1289 CE MET 188 1852 2032 2855 -242 505 1 2 1
 ATOM 1290 N VAL 189 12.244 17.112 44.616 1.000 12.62
 ANISOU 1290 N VAL 189 1586 1203 2007 103 -147 -1 3 4
 ATOM 1291 CA VAL 189 12.565 17.671 45.918 1.000 12.60
 ANISOU 1291 CA VAL 189 1412 1438 1937 -228 -11 -4 4
 ATOM 1292 C VAL 189 11.285 17.968 46.679 1.000 11.71
 ANISOU 1292 C VAL 189 1328 1294 1825 -170 -171 -4 9
 ATOM 1293 O VAL 189 10.227 18.099 46.050 1.000 12.56
 ANISOU 1293 O VAL 189 1446 1291 2036 21 -320 -4 9
 ATOM 1294 CB VAL 189 13.440 18.955 45.856 1.000 12.95
 ANISOU 1294 CB VAL 189 1150 1517 2252 -174 -205 9 4
 ATOM 1295 CG1 VAL 189 14.778 18.637 45.167 1.000 15.54
 ANISOU 1295 CG1 VAL 189 1376 2094 2437 -140 161 9 1
 ATOM 1296 CG2 VAL 189 12.730 20.056 45.082 1.000 15.00
 ANISOU 1296 CG2 VAL 189 1763 1391 2547 -130 -483 8 1
 ATOM 1297 N THR 190 11.425 18.067 47.984 1.000 12.18
 ANISOU 1297 N THR 190 1445 1422 1760 -109 -130 1 0
 ATOM 1298 CA THR 190 10.353 18.454 48.897 1.000 11.98
 ANISOU 1298 CA THR 190 1292 1356 1903 -57 -221 -1 5 1
 ATOM 1299 C THR 190 10.879 19.630 49.710 1.000 12.47
 ANISOU 1299 C THR 190 1178 1436 2124 -32 -297 -2 3 2
 ATOM 1300 O THR 190 11.959 19.523 50.320 1.000 15.06
 ANISOU 1300 O THR 190 1424 1767 2531 46 -571 -4 4 6
 ATOM 1301 CB THR 190 9.913 17.297 49.808 1.000 13.16
 ANISOU 1301 CB THR 190 1509 1605 1886 -168 80 -1 2 1
 ATOM 1302 OG1 THR 190 9.481 16.201 48.993 1.000 14.47
 ANISOU 1302 OG1 THR 190 1693 1469 2334 -100 -25 -1 9 4
 ATOM 1303 CG2 THR 190 8.778 17.723 50.734 1.000 14.79
 ANISOU 1303 CG2 THR 190 1696 1510 2415 73 258 -8 9
 ATOM 1304 N LEU 191 10.148 20.724 49.732 1.000 12.97
 ANISOU 1304 N LEU 191 1329 1449 2149 23 -21 -2 8 6
 ATOM 1305 CA LEU 191 10.511 21.908 50.526 1.000 13.75
 ANISOU 1305 CA LEU 191 1543 1442 2238 78 -206 -3 0 1
 ATOM 1306 C LEU 191 9.603 21.964 51.763 1.000 14.47
 ANISOU 1306 C LEU 191 1543 1689 2265 83 -179 -4 1 2
 ATOM 1307 O LEU 191 8.370 21.868 51.645 1.000 16.58
 ANISOU 1307 O LEU 191 1517 2486 2297 219 -176 -7 2 5
 ATOM 1308 CB LEU 191 10.398 23.212 49.722 1.000 15.37
 ANISOU 1308 CB LEU 191 1717 1444 2680 58 -106 -1 8 9
 ATOM 1309 CG LEU 191 11.705 23.578 48.973 1.000 16.10
 ANISOU 1309 CG LEU 191 1747 1688 2680 -128 -113 -1 3 5
 ATOM 1310 CD1 LEU 191 12.069 22.565 47.906 1.000 16.67
 ANISOU 1310 CD1 LEU 191 2034 2093 2209 -23 -64 1 9
 ATOM 1311 CD2 LEU 191 11.570 24.959 48.350 1.000 18.53
 ANISOU 1311 CD2 LEU 191 2297 1906 2837 -345 -437 1 4 8
 ATOM 1312 N ILE 192 10.199 22.148 52.946 1.000 15.36

- 56 -

ANISOU	1312	N	ILE	192	1479	2152	2204	-47	-165	-164
ATOM	1313	CA	ILE	192	9.417	22.162	54.194	1.000	15.13	
ANISOU	1313	CA	ILE	192	1456	2043	2251	-304	-173	-280
ATOM	1314	C	ILE	192	9.692	23.423	55.010	1.000	15.58	
ANISOU	1314	C	ILE	192	1696	1973	2251	-199	-254	-226
ATOM	1315	O	ILE	192	10.836	23.691	55.381	1.000	17.20	
ANISOU	1315	O	ILE	192	1856	2449	2229	-307	-341	-574
ATOM	1316	CB	ILE	192	9.722	20.920	55.040	1.000	17.03	
ANISOU	1316	CB	ILE	192	2246	1958	2266	-52	325	-303
ATOM	1317	CG1	ILE	192	9.454	19.596	54.317	1.000	19.80	
ANISOU	1317	CG1	ILE	192	3040	2010	2473	-71	128	-382
ATOM	1318	CG2	ILE	192	8.995	20.967	56.403	1.000	18.14	
ANISOU	1318	CG2	ILE	192	2278	2354	2262	229	290	-258
ATOM	1319	CD1	ILE	192	9.420	18.387	55.235	1.000	31.57	
ANISOU	1319	CD1	ILE	192	4658	2114	5222	-398	-1094	765
ATOM	1320	N	GLN	193	8.625	24.172	55.249	1.000	17.04	
ANISOU	1320	N	GLN	193	2042	2185	2248	112	-388	-301
ATOM	1321	CA	GLN	193	8.680	25.291	56.201	1.000	17.70	
ANISOU	1321	CA	GLN	193	1737	2167	2824	-204	-186	-559
ATOM	1322	C	GLN	193	7.898	24.869	57.443	1.000	19.67	
ANISOU	1322	C	GLN	193	1882	2624	2969	-232	211	-840
ATOM	1323	O	GLN	193	7.082	23.942	57.426	1.000	26.60	
ANISOU	1323	O	GLN	193	2066	3843	4197	-965	-110	62
ATOM	1324	CB	GLN	193	8.129	26.598	55.643	1.000	23.74	
ANISOU	1324	CB	GLN	193	3070	2388	3561	500	-98	-514
ATOM	1325	CG	GLN	193	8.913	27.304	54.559	1.000	28.26	
ANISOU	1325	CG	GLN	193	4664	2384	3689	656	209	0
ATOM	1326	CD	GLN	193	8.338	28.665	54.156	1.000	26.30	
ANISOU	1326	CD	GLN	193	2868	2943	4181	791	3	111
ATOM	1327	OE1	GLN	193	7.193	28.695	53.688	1.000	45.31	
ANISOU	1327	OE1	GLN	193	2826	7147	7241	-51	-616	3173
ATOM	1328	NE2	GLN	193	9.080	29.748	54.345	1.000	30.44	
ANISOU	1328	NE2	GLN	193	3609	2588	5368	418	1259	692
ATOM	1329	N	GLN	194	8.241	25.259	58.645	1.000	22.04	
ANISOU	1329	N	GLN	194	2926	2758	2690	303	-368	-83
ATOM	1330	CA	GLN	194	7.569	24.793	59.847	1.000	22.68	
ANISOU	1330	CA	GLN	194	3144	2617	2855	82	-230	-150
ATOM	1331	C	GLN	194	7.275	26.054	60.663	1.000	22.19	
ANISOU	1331	C	GLN	194	2809	2768	2856	117	-396	-320
ATOM	1332	O	GLN	194	7.889	27.100	60.418	1.000	25.26	
ANISOU	1332	O	GLN	194	4041	2877	2679	-313	-21	-411
ATOM	1333	CB	GLN	194	8.467	23.943	60.739	1.000	29.21	
ANISOU	1333	CB	GLN	194	4493	2707	3899	477	-50	939
ATOM	1334	CG	GLN	194	9.105	22.735	60.083	1.000	28.80	
ANISOU	1334	CG	GLN	194	3108	3530	4305	576	-121	494
ATOM	1335	CD	GLN	194	10.296	22.332	60.962	1.000	31.97	
ANISOU	1335	CD	GLN	194	2961	5384	3800	824	359	1075
ATOM	1336	OE1	GLN	194	11.421	22.325	60.474	1.000	27.28	
ANISOU	1336	OE1	GLN	194	2781	4189	3397	118	133	-249
ATOM	1337	NE2	GLN	194	9.998	22.100	62.232	1.000	29.82	
ANISOU	1337	NE2	GLN	194	3540	3958	3832	989	645	800
ATOM	1338	N	THR	195	6.419	25.891	61.658	1.000	23.30	
ANISOU	1338	N	THR	195	2407	3058	3387	-211	-235	-720
ATOM	1339	CA	THR	195	6.476	26.833	62.768	1.000	27.14	
ANISOU	1339	CA	THR	195	3459	3544	3308	25	-50	-890
ATOM	1340	C	THR	195	6.933	25.997	63.958	1.000	26.11	
ANISOU	1340	C	THR	195	3825	2829	3268	558	19	-1247
ATOM	1341	O	THR	195	6.639	24.815	63.994	1.000	28.17	
ANISOU	1341	O	THR	195	2973	2916	4815	481	171	-1030
ATOM	1342	CB	THR	195	5.149	27.534	63.069	1.000	25.87	
ANISOU	1342	CB	THR	195	3428	2849	3551	-16	-592	-1137

- 57 -

ATOM	1343	OG1	THR	195	4.111	26.550	63.196	1.000	25.45
ANISOU	1343	OG1	THR	195	3427	3101	3141	-9	-117 -750
ATOM	1344	CG2	THR	195	4.788	28.396	61.847	1.000	31.31
ANISOU	1344	CG2	THR	195	4965	2552	4380	274	-70 -409
ATOM	1345	N	PRO	196	7.604	26.587	64.923	1.000	30.84
ANISOU	1345	N	PRO	196	5225	3191	3300	785	-517 -1542
ATOM	1346	CA	PRO	196	8.101	25.823	66.065	1.000	28.50
ANISOU	1346	CA	PRO	196	3113	3700	4016	-279	-441 -646
ATOM	1347	C	PRO	196	7.018	25.534	67.096	1.000	28.97
ANISOU	1347	C	PRO	196	3581	3326	4102	42	113 -1381
ATOM	1348	O	PRO	196	6.002	26.229	67.192	1.000	32.32
ANISOU	1348	O	PRO	196	4146	4649	3485	901	-180 -1658
ATOM	1349	CB	PRO	196	9.094	26.816	66.694	1.000	29.72
ANISOU	1349	CB	PRO	196	3888	3292	4111	-285	-353 -1072
ATOM	1350	CG	PRO	196	8.533	28.174	66.364	1.000	34.87
ANISOU	1350	CG	PRO	196	6285	3575	3390	421	-1326 -1332
ATOM	1351	CD	PRO	196	7.897	28.035	65.012	1.000	33.20
ANISOU	1351	CD	PRO	196	6407	3606	2600	-598	-494 -1031
ATOM	1352	N	CYS	197	7.289	24.533	67.919	1.000	26.96
ANISOU	1352	N	CYS	197	2739	4038	3465	-113	85 -1227
ATOM	1353	CA	CYS	197	6.519	24.289	69.126	1.000	31.73
ANISOU	1353	CA	CYS	197	3979	4543	3533	-39	721 -1726
ATOM	1354	C	CYS	197	6.803	25.412	70.124	1.000	35.58
ANISOU	1354	C	CYS	197	4213	4819	4486	-480	1126 -2282
ATOM	1355	O	CYS	197	7.917	25.939	70.175	1.000	31.34
ANISOU	1355	O	CYS	197	3817	4845	3246	36	-383 -992
ATOM	1356	CB	CYS	197	6.940	22.962	69.767	1.000	35.79
ANISOU	1356	CB	CYS	197	5913	4705	2980	284	1566 -1423
ATOM	1357	SG	CYS	197	6.553	21.535	68.741	1.000	28.53
ANISOU	1357	SG	CYS	197	3605	4224	3009	50	-5 -452
ATOM	1358	N	ALA	198	5.771	25.791	70.866	1.000	37.27
ANISOU	1358	N	ALA	198	5038	4984	4139	-421	1647 -2070
ATOM	1359	CA	ALA	198	5.983	26.811	71.888	1.000	35.91
ANISOU	1359	CA	ALA	198	6273	4144	3230	910	522 -1230
ATOM	1360	C	ALA	198	6.993	26.328	72.921	1.000	44.30
ANISOU	1360	C	ALA	198	5998	6138	4696	-193	-199 3
ATOM	1361	O	ALA	198	7.759	27.127	73.457	1.000	42.85
ANISOU	1361	O	ALA	198	5209	6328	4742	7	490 -555
ATOM	1362	CB	ALA	198	4.671	27.231	72.532	1.000	41.70
ANISOU	1362	CB	ALA	198	7588	5697	2557	2355	1068 -721
ATOM	1363	N	ASN	199	7.036	25.036	73.225	1.000	34.93
ANISOU	1363	N	ASN	199	4027	5975	3270	805	167 -621
ATOM	1364	CA	ASN	199	7.969	24.578	74.264	1.000	33.58
ANISOU	1364	CA	ASN	199	3643	6167	2950	-670	-265 -808
ATOM	1365	C	ASN	199	9.352	24.262	73.718	1.000	31.53
ANISOU	1365	C	ASN	199	4077	5048	2853	384	-420 -855
ATOM	1366	O	ASN	199	10.153	23.667	74.467	1.000	36.33
ANISOU	1366	O	ASN	199	4223	5624	3957	-403	-1305 -126
ATOM	1367	CB	ASN	199	7.441	23.308	74.929	1.000	36.38
ANISOU	1367	CB	ASN	199	4533	5029	4262	859	584 -522
ATOM	1368	CG	ASN	199	7.198	22.180	73.952	1.000	31.28
ANISOU	1368	CG	ASN	199	4030	4863	2993	882	202 178
ATOM	1369	OD1	ASN	199	7.743	22.151	72.853	1.000	37.62
ANISOU	1369	OD1	ASN	199	4693	6272	3330	122	728 -56
ATOM	1370	ND2	ASN	199	6.393	21.190	74.314	1.000	36.42
ANISOU	1370	ND2	ASN	199	3508	6251	4078	-13	1132 -958
ATOM	1371	N	GLY	200	9.616	24.569	72.449	1.000	30.93
ANISOU	1371	N	GLY	200	4342	4232	3179	436	144 -692
ATOM	1372	CA	GLY	200	10.920	24.304	71.866	1.000	35.26
ANISOU	1372	CA	GLY	200	4430	4905	4060	-317	480 -2400
ATOM	1373	C	GLY	200	11.184	22.886	71.429	1.000	36.83

- 58 -

ANISOU	1373	C	GLY	200	4683	4375	4936	-360	1601	-1460
ATOM	1374	O	GLY	200	12.257	22.566	70.897	1.000	32.71	
ANISOU	1374	O	GLY	200	3921	4072	4436	-377	752	-1400
ATOM	1375	N	PHE	201	10.264	21.939	71.588	1.000	28.66	
ANISOU	1375	N	PHE	201	3813	4229	2847	145	463	-326
ATOM	1376	CA	PHE	201	10.491	20.575	71.106	1.000	27.55	
ANISOU	1376	CA	PHE	201	3190	4337	2943	-233	219	-672
ATOM	1377	C	PHE	201	10.752	20.553	69.600	1.000	24.89	
ANISOU	1377	C	PHE	201	2943	3682	2832	190	-268	-379
ATOM	1378	O	PHE	201	9.994	21.255	68.910	1.000	28.22	
ANISOU	1378	O	PHE	201	3583	3184	3957	10	-421	277
ATOM	1379	CB	PHE	201	9.250	19.729	71.413	1.000	30.46	
ANISOU	1379	CB	PHE	201	3153	4862	3560	-371	-40	-73
ATOM	1380	CG	PHE	201	9.425	18.262	71.027	1.000	34.89	
ANISOU	1380	CG	PHE	201	4015	4609	4632	-772	162	89
ATOM	1381	CD1	PHE	201	10.395	17.472	71.605	1.000	31.18	
ANISOU	1381	CD1	PHE	201	3436	4103	4310	-875	-93	-1105
ATOM	1382	CD2	PHE	201	8.613	17.681	70.078	1.000	28.84	
ANISOU	1382	CD2	PHE	201	2979	4019	3960	329	612	-107
ATOM	1383	CE1	PHE	201	10.564	16.160	71.240	1.000	37.73	
ANISOU	1383	CE1	PHE	201	6489	3608	4239	-1078	-1475	-500
ATOM	1384	CE2	PHE	201	8.761	16.363	69.679	1.000	31.78	
ANISOU	1384	CE2	PHE	201	4327	3911	3838	652	250	119
ATOM	1385	CZ	PHE	201	9.755	15.606	70.265	1.000	29.78	
ANISOU	1385	CZ	PHE	201	3705	3397	4211	6	-638	-849
ATOM	1386	N	VAL	202	11.706	19.751	69.144	1.000	23.51	
ANISOU	1386	N	VAL	202	2671	3392	2868	-292	-1	-578
ATOM	1387	CA	VAL	202	11.969	19.626	67.706	1.000	26.37	
ANISOU	1387	CA	VAL	202	3025	4050	2946	-667	57	-724
ATOM	1388	C	VAL	202	11.423	18.283	67.198	1.000	22.75	
ANISOU	1388	C	VAL	202	2729	3348	2567	96	-120	-435
ATOM	1389	O	VAL	202	11.880	17.190	67.541	1.000	28.71	
ANISOU	1389	O	VAL	202	3249	3799	3859	119	31	661
ATOM	1390	CB	VAL	202	13.476	19.721	67.415	1.000	24.99	
ANISOU	1390	CB	VAL	202	3060	3427	3008	-278	283	152
ATOM	1391	CG1	VAL	202	13.715	19.464	65.938	1.000	27.70	
ANISOU	1391	CG1	VAL	202	4642	2577	3307	87	1014	-3
ATOM	1392	CG2	VAL	202	14.050	21.071	67.823	1.000	26.80	
ANISOU	1392	CG2	VAL	202	2826	3868	3487	-490	474	-398
ATOM	1393	N	SER	203	10.405	18.402	66.333	1.000	24.10	
ANISOU	1393	N	SER	203	2194	3607	3356	-31	-179	-528
ATOM	1394	CA	SER	203	9.634	17.231	65.940	1.000	23.70	
ANISOU	1394	CA	SER	203	2373	3584	3046	-290	308	-533
ATOM	1395	C	SER	203	10.168	16.511	64.710	1.000	21.28	
ANISOU	1395	C	SER	203	2173	3041	2871	46	227	-42
ATOM	1396	O	SER	203	10.159	15.285	64.640	1.000	27.60	
ANISOU	1396	O	SER	203	4105	3097	3284	-482	1010	-249
ATOM	1397	CB	SER	203	8.148	17.571	65.685	1.000	29.06	
ANISOU	1397	CB	SER	203	2251	3790	5001	-180	203	-2064
ATOM	1398	OG	SER	203	7.584	18.175	66.843	1.000	32.55	
ANISOU	1398	OG	SER	203	3840	4298	4231	920	1099	-382
ATOM	1399	N	LEU	204	10.688	17.233	63.724	1.000	22.46	
ANISOU	1399	N	LEU	204	2476	3013	3043	79	450	-46
ATOM	1400	CA	LEU	204	11.166	16.530	62.544	1.000	20.26	
ANISOU	1400	CA	LEU	204	2200	2831	2667	45	-18	-15
ATOM	1401	C	LEU	204	12.595	16.038	62.747	1.000	18.83	
ANISOU	1401	C	LEU	204	2151	2528	2477	-75	60	-1
ATOM	1402	O	LEU	204	13.443	16.783	63.251	1.000	20.47	
ANISOU	1402	O	LEU	204	2333	2386	3059	-303	-195	404
ATOM	1403	CB	LEU	204	11.103	17.486	61.362	1.000	21.42	
ANISOU	1403	CB	LEU	204	2718	2548	2871	311	-16	-8

- 59 -

ATOM 1404 CG LEU 204 9.769 18.188 61.079 1.000 33.57
 ANISOU 1404 CG LEU 204 2820 4319 5617 177 -1316 1 1 7 2
 ATOM 1405 CD1 LEU 204 9.797 18.747 59.660 1.000 36.19
 ANISOU 1405 CD1 LEU 204 4402 3807 5540 1276 -1167 9 8 7
 ATOM 1406 CD2 LEU 204 8.581 17.234 61.219 1.000 37.76
 ANISOU 1406 CD2 LEU 204 3058 5328 5960 -526 -1896 6 8 6
 ATOM 1407 N GLN 205 12.864 14.836 62.284 1.000 20.33
 ANISOU 1407 N GLN 205 2518 2644 2563 104 -31 -1 2 9
 ATOM 1408 CA GLN 205 14.209 14.247 62.335 1.000 18.88
 ANISOU 1408 CA GLN 205 2522 2225 2425 -6 -181 3 6
 ATOM 1409 C GLN 205 14.512 13.504 61.036 1.000 18.19
 ANISOU 1409 C GLN 205 1986 2383 2543 -143 -188 -8 0
 ATOM 1410 O GLN 205 13.577 13.033 60.408 1.000 19.87
 ANISOU 1410 O GLN 205 1974 3063 2514 -125 -212 -2 3 7
 ATOM 1411 CB GLN 205 14.296 13.267 63.493 1.000 24.25
 ANISOU 1411 CB GLN 205 3948 2716 2548 202 -343 2 9 6
 ATOM 1412 CG GLN 205 14.164 13.948 64.856 1.000 30.64
 ANISOU 1412 CG GLN 205 4099 5159 2382 850 -327 -8 9
 ATOM 1413 CD GLN 205 14.744 13.078 65.948 1.000 28.28
 ANISOU 1413 CD GLN 205 4473 3633 2640 -161 -1015 -3 9 0
 ATOM 1414 OE1 GLN 205 14.307 11.921 66.041 1.000 37.69
 ANISOU 1414 OE1 GLN 205 5733 5073 3515 -2145 -699 4 7 8
 ATOM 1415 NE2 GLN 205 15.710 13.553 66.711 1.000 40.53
 ANISOU 1415 NE2 GLN 205 6798 4417 4185 -1341 -2865 3 2 3
 ATOM 1416 N ALA 206 15.752 13.471 60.576 1.000 18.52
 ANISOU 1416 N ALA 206 2070 2199 2769 -240 -13 4
 ATOM 1417 CA ALA 206 16.152 12.700 59.405 1.000 18.42
 ANISOU 1417 CA ALA 206 2074 2351 2575 -100 -158 2 3
 ATOM 1418 C ALA 206 17.343 11.802 59.738 1.000 17.41
 ANISOU 1418 C ALA 206 2107 2158 2350 -185 -254 -1 7
 ATOM 1419 O ALA 206 18.123 12.203 60.613 1.000 20.67
 ANISOU 1419 O ALA 206 2469 2410 2973 -48 -711 -3 9 6
 ATOM 1420 CB ALA 206 16.637 13.599 58.270 1.000 18.77
 ANISOU 1420 CB ALA 206 2119 2310 2703 156 -65 1 4 7
 ATOM 1421 N GLU 207 17.492 10.764 58.931 1.000 18.09
 ANISOU 1421 N GLU 207 2092 2101 2680 -249 -496 -1 6 2
 ATOM 1422 CA GLU 207 18.710 9.944 58.966 1.000 19.48
 ANISOU 1422 CA GLU 207 2210 2091 3100 -73 -432 -4 4
 ATOM 1423 C GLU 207 19.851 10.730 58.320 1.000 19.98
 ANISOU 1423 C GLU 207 2018 2233 3342 220 -560 5 4 4
 ATOM 1424 O GLU 207 19.732 11.068 57.143 1.000 20.33
 ANISOU 1424 O GLU 207 2000 2753 2970 5 -471 8 9
 ATOM 1425 CB GLU 207 18.566 8.623 58.214 1.000 24.03
 ANISOU 1425 CB GLU 207 3401 1784 3946 316 -1226 6 1
 ATOM 1426 CG GLU 207 19.757 7.674 58.295 1.000 24.35
 ANISOU 1426 CG GLU 207 3223 1907 4121 354 93 4 6 7
 ATOM 1427 CD GLU 207 20.730 7.791 57.129 1.000 31.69
 ANISOU 1427 CD GLU 207 2729 5178 4134 -1218 -175 1 2 2
 ATOM 1428 OE1 GLU 207 20.376 7.611 55.943 1.000 26.97
 ANISOU 1428 OE1 GLU 207 2849 3404 3993 31 -256 3 0 9
 ATOM 1429 OE2 GLU 207 21.908 8.121 57.407 1.000 30.70
 ANISOU 1429 OE2 GLU 207 2484 3416 5764 -233 -342 -1 1 6 8
 ATOM 1430 N VAL 208 20.919 10.936 59.078 1.000 18.53
 ANISOU 1430 N VAL 208 2020 2112 2907 130 -362 3 2 0
 ATOM 1431 CA VAL 208 22.150 11.547 58.541 1.000 19.53
 ANISOU 1431 CA VAL 208 2044 2238 3137 39 -476 6 3 0
 ATOM 1432 C VAL 208 23.341 10.755 59.088 1.000 21.95
 ANISOU 1432 C VAL 208 2040 2792 3507 225 -461 7 9 7
 ATOM 1433 O VAL 208 23.460 10.663 60.314 1.000 23.82
 ANISOU 1433 O VAL 208 2262 3240 3547 -40 -858 8 2 5
 ATOM 1434 CB VAL 208 22.271 13.027 58.905 1.000 19.72

- 60 -

ANISOU	1434	CB	VAL	208	1918	2429	3145	-47	-308	3	1	1
ATOM	1435	CG1	VAL	208	23.524	13.626	58.281	1.000	23.1	4		
ANISOU	1435	CG1	VAL	208	2524	2374	3895	-202	284	3	4	9
ATOM	1436	CG2	VAL	208	21.030	13.812	58.469	1.000	19.4	7		
ANISOU	1436	CG2	VAL	208	2462	2279	2658	232	-667	-	8	7
ATOM	1437	N	GLY	209	24.180	10.169	58.246	1.000	23.88			
ANISOU	1437	N	GLY	209	2500	2449	4123	465	-711	3	6	
ATOM	1438	CA	GLY	209	25.306	9.374	58.773	1.000	26.42			
ANISOU	1438	CA	GLY	209	1987	3599	4450	460	-487	5	1	6
ATOM	1439	C	GLY	209	24.905	8.250	59.695	1.000	30.01			
ANISOU	1439	C	GLY	209	3469	3240	4693	238	-1422	7	3	2
ATOM	1440	O	GLY	209	25.609	7.835	60.629	1.000	31.45			
ANISOU	1440	O	GLY	209	4053	4458	3438	1225	-897	8	3	
ATOM	1441	N	GLY	210	23.691	7.702	59.523	1.000	26.64			
ANISOU	1441	N	GLY	210	3165	3214	3744	259	-86	3	5	0
ATOM	1442	CA	GLY	210	23.263	6.585	60.360	1.000	29.78			
ANISOU	1442	CA	GLY	210	4603	3091	3619	-55	-997	5	8	4
ATOM	1443	C	GLY	210	22.622	6.993	61.663	1.000	38.28			
ANISOU	1443	C	GLY	210	5827	4212	4507	-2536	732	5	0	
ATOM	1444	O	GLY	210	22.160	6.187	62.481	1.000	41.45			
ANISOU	1444	O	GLY	210	4152	6516	5082	-1874	-567	2	3	4
ATOM	1445	N	ALA	211	22.512	8.274	61.976	1.000	32.81			
ANISOU	1445	N	ALA	211	4803	4625	3037	1372	-1177	6	3	2
ATOM	1446	CA	ALA	211	21.828	8.603	63.235	1.000	35.62			
ANISOU	1446	CA	ALA	211	3993	5958	3584	1061	-610	9	7	0
ATOM	1447	C	ALA	211	20.663	9.543	62.940	1.000	31.43			
ANISOU	1447	C	ALA	211	3508	4737	3699	302	69	1	8	5
ATOM	1448	O	ALA	211	20.652	10.097	61.858	1.000	28.28			
ANISOU	1448	O	ALA	211	3661	4062	3020	-571	-551	1	0	1
ATOM	1449	CB	ALA	211	22.812	9.278	64.170	1.000	41.36			
ANISOU	1449	CB	ALA	211	3644	8904	3169	1372	-18	-	7	9
ATOM	1450	N	PHE	212	19.682	9.676	63.825	1.000	36.68			
ANISOU	1450	N	PHE	212	5211	4237	4489	1166	1265	2	1	7
ATOM	1451	CA	PHE	212	18.620	10.654	63.641	1.000	28.82			
ANISOU	1451	CA	PHE	212	4490	3167	3293	263	504	1	0	3
ATOM	1452	C	PHE	212	19.100	12.023	64.124	1.000	34.72			
ANISOU	1452	C	PHE	212	6746	3760	2685	-248	-539	7	7	6
ATOM	1453	O	PHE	212	19.667	12.191	65.210	1.000	39.12			
ANISOU	1453	O	PHE	212	6144	5384	3335	-549	-1129	1	2	2
ATOM	1454	CB	PHE	212	17.358	10.219	64.388	1.000	45.35			
ANISOU	1454	CB	PHE	212	6376	2569	8288	1348	3748	2	3	1
ATOM	1455	N	THR	213	18.906	13.008	63.271	1.000	26.30			
ANISOU	1455	N	THR	213	4134	2738	3122	662	-581	1	0	0
ATOM	1456	CA	THR	213	19.424	14.359	63.433	1.000	25.08			
ANISOU	1456	CA	THR	213	3587	2852	3089	767	-810	-	3	2
ATOM	1457	C	THR	213	18.190	15.283	63.400	1.000	23.81			
ANISOU	1457	C	THR	213	2835	2652	3560	215	-855	-	6	4
ATOM	1458	O	THR	213	17.329	15.137	62.517	1.000	21.40			
ANISOU	1458	O	THR	213	2640	2269	3223	-328	-580	-	1	7
ATOM	1459	CB	THR	213	20.398	14.759	62.308	1.000	27.60			
ANISOU	1459	CB	THR	213	3155	3220	4113	189	-356	-	7	9
ATOM	1460	OG1	THR	213	21.673	14.084	62.374	1.000	32.00			
ANISOU	1460	OG1	THR	213	3582	4220	4356	746	-410	5	2	0
ATOM	1461	CG2	THR	213	20.735	16.254	62.355	1.000	29.45			
ANISOU	1461	CG2	THR	213	4422	3320	3448	-106	-1265	-	2	0
ATOM	1462	N	ASP	214	18.119	16.177	64.371	1.000	21.05			
ANISOU	1462	N	ASP	214	2790	2236	2972	-82	-380	-	1	4
ATOM	1463	CA	ASP	214	17.001	17.110	64.462	1.000	20.61			
ANISOU	1463	CA	ASP	214	2742	2095	2993	-117	-898	-	3	7
ATOM	1464	C	ASP	214	16.994	18.030	63.226	1.000	20.58			
ANISOU	1464	C	ASP	214	2373	2525	2923	182	-169	-	2	3

- 61 -

ATOM 1465 O ASP 214 18.018 18.430 62.678 1.000 23.02
 ANISOU 1465 O ASP 214 2461 2883 3404 -167 -52 -5 7 2
 ATOM 1466 CB ASP 214 17.205 18.058 65.637 1.000 23.54
 ANISOU 1466 CB ASP 214 3304 2607 3032 -92 -748 -6 6 8
 ATOM 1467 CG ASP 214 16.915 17.506 67.004 1.000 24.93
 ANISOU 1467 CG ASP 214 3545 2850 3079 450 -417 -6 1 4
 ATOM 1468 OD1 ASP 214 16.357 16.395 67.113 1.000 29.17
 ANISOU 1468 OD1 ASP 214 4134 3070 3878 202 -705 2 6 2
 ATOM 1469 OD2 ASP 214 17.276 18.191 67.990 1.000 34.38
 ANISOU 1469 OD2 ASP 214 6917 3040 3107 1017 -1413 -7 3 6
 ATOM 1470 N LEU 215 15.802 18.452 62.859 1.000 20.74
 ANISOU 1470 N LEU 215 2426 2372 3081 86 -60 3 0 6
 ATOM 1471 CA LEU 215 15.568 19.401 61.796 1.000 20.55
 ANISOU 1471 CA LEU 215 2895 2013 2899 -202 -178 1 4 1
 ATOM 1472 C LEU 215 14.724 20.552 62.332 1.000 19.02
 ANISOU 1472 C LEU 215 2482 2240 2504 -142 -34 3 2 1
 ATOM 1473 O LEU 215 13.510 20.613 62.142 1.000 22.39
 ANISOU 1473 O LEU 215 2635 2483 3389 -160 -475 5 7 3
 ATOM 1474 CB LEU 215 14.826 18.722 60.650 1.000 22.04
 ANISOU 1474 CB LEU 215 2778 2510 3086 -140 -261 -6 5
 ATOM 1475 CG LEU 215 15.598 17.502 60.128 1.000 25.25
 ANISOU 1475 CG LEU 215 3680 2829 3085 85 -166 -4 0 2
 ATOM 1476 CD1 LEU 215 14.680 16.736 59.174 1.000 27.12
 ANISOU 1476 CD1 LEU 215 4886 2934 2482 419 -1128 -6 5
 ATOM 1477 CD2 LEU 215 16.881 18.046 59.510 1.000 30.76
 ANISOU 1477 CD2 LEU 215 3434 3089 5165 1003 524 5 6 1
 ATOM 1478 N PRO 216 15.383 21.433 63.078 1.000 19.68
 ANISOU 1478 N PRO 216 2407 2191 2879 -157 148 1 0 3
 ATOM 1479 CA PRO 216 14.665 22.534 63.708 1.000 22.42
 ANISOU 1479 CA PRO 216 2869 2812 2836 272 10 -2 2 8
 ATOM 1480 C PRO 216 14.201 23.576 62.698 1.000 25.36
 ANISOU 1480 C PRO 216 4118 2433 3086 566 -131 -3 1 5
 ATOM 1481 O PRO 216 14.700 23.759 61.586 1.000 24.67
 ANISOU 1481 O PRO 216 3682 2406 3284 187 -176 -2 6
 ATOM 1482 CB PRO 216 15.693 23.092 64.676 1.000 23.88
 ANISOU 1482 CB PRO 216 3108 3049 2917 -216 116 -3 1 8
 ATOM 1483 CG PRO 216 17.033 22.701 64.146 1.000 28.31
 ANISOU 1483 CG PRO 216 2994 2996 4766 -88 -117 -1 4 5 4
 ATOM 1484 CD PRO 216 16.807 21.405 63.436 1.000 24.55
 ANISOU 1484 CD PRO 216 2353 1777 5197 -436 -83 -3 4 8
 ATOM 1485 N TYR 217 13.154 24.287 63.102 1.000 24.13
 ANISOU 1485 N TYR 217 3237 2704 3229 244 -631 -5 1 1
 ATOM 1486 CA TYR 217 12.676 25.510 62.462 1.000 26.08
 ANISOU 1486 CA TYR 217 2514 2899 4498 104 -592 3 9
 ATOM 1487 C TYR 217 13.824 26.516 62.369 1.000 25.24
 ANISOU 1487 C TYR 217 3049 2948 3592 -257 -506 -5 3 8
 ATOM 1488 O TYR 217 14.570 26.675 63.340 1.000 31.78
 ANISOU 1488 O TYR 217 4114 2863 5096 -352 -2151 5 6 4
 ATOM 1489 CB TYR 217 11.559 26.103 63.315 1.000 25.97
 ANISOU 1489 CB TYR 217 2747 2773 4346 86 -615 -1 6 7
 ATOM 1490 CG TYR 217 11.189 27.543 63.125 1.000 31.64
 ANISOU 1490 CG TYR 217 3080 2803 6139 338 -1473 -6 4 4
 ATOM 1491 CD1 TYR 217 10.430 27.928 62.022 1.000 27.85
 ANISOU 1491 CD1 TYR 217 2238 3029 5314 511 -175 9 3
 ATOM 1492 CD2 TYR 217 11.512 28.522 64.069 1.000 38.49
 ANISOU 1492 CD2 TYR 217 4721 2813 7093 -686 -1682 -7 4 9
 ATOM 1493 CE1 TYR 217 10.021 29.219 61.772 1.000 26.53
 ANISOU 1493 CE1 TYR 217 1908 2675 5496 -41 107 6 9
 ATOM 1494 CE2 TYR 217 11.113 29.835 63.827 1.000 42.90
 ANISOU 1494 CE2 TYR 217 7112 2347 6842 -1415 -1949 -2 1 8
 ATOM 1495 CZ TYR 217 10.373 30.168 62.712 1.000 34.93

- 62 -

ANISOU	1495	CZ	TYR	217	4042	2747	6483	-1462	-545	1	6	6
ATOM	1496	OH	TYR	217	9.996	31.486	62.473	1.000	36.41			
ANISOU	1496	OH	TYR	217	5499	2895	5439	-753	-250	-2	8	9
ATOM	1497	N	ARG	218	14.022	27.110	61.218	1.000	25.58			
ANISOU	1497	N	ARG	218	3461	2406	3852	-227	-533	-4	7	6
ATOM	1498	CA	ARG	218	14.923	28.243	61.049	1.000	29.26			
ANISOU	1498	CA	ARG	218	3630	3270	4219	-784	-1349	2	6	8
ATOM	1499	C	ARG	218	14.113	29.336	60.366	1.000	24.81			
ANISOU	1499	C	ARG	218	4063	2949	2415	-382	-228	-5	6	
ATOM	1500	O	ARG	218	13.746	29.174	59.212	1.000	29.56			
ANISOU	1500	O	ARG	218	6298	2267	2666	-890	-994	1	6	5
ATOM	1501	CB	ARG	218	16.162	27.823	60.256	1.000	35.90			
ANISOU	1501	CB	ARG	218	3223	3685	6732	-624	-703	8	9	6
ATOM	1502	CG	ARG	218	17.369	28.665	60.661	1.000	51.38			
ANISOU	1502	CG	ARG	218	4740	6768	8015	-3031	430	-1	8	3
ATOM	1503	CD	ARG	218	18.539	28.606	59.701	1.000	38.84			
ANISOU	1503	CD	ARG	218	4968	6308	3482	-3596	-1165	1	6	4
ATOM	1504	NE	ARG	218	19.343	27.395	59.905	1.000	45.09			
ANISOU	1504	NE	ARG	218	4655	7495	4982	-2325	-962	-9	4	
ATOM	1505	CZ	ARG	218	20.272	27.208	58.959	1.000	55.53			
ANISOU	1505	CZ	ARG	218	5299	11458	4340	-2701	-1188	-1	9	4
ATOM	1506	NH1	ARG	218	20.289	28.158	58.031	1.000	60.85			
ANISOU	1506	NH1	ARG	218	2399	16648	4071	-1943	-1333	5	4	8
ATOM	1507	NH2	ARG	218	21.060	26.165	59.001	1.000	60.37			
ANISOU	1507	NH2	ARG	218	8580	10111	4247	-2152	639	-4	2	4
ATOM	1508	N	PRO	219	13.871	30.496	60.972	1.000	25.89			
ANISOU	1508	N	PRO	219	2625	4126	3086	35	296	-1	0	1
ATOM	1509	CA	PRO	219	13.065	31.548	60.326	1.000	28.10			
ANISOU	1509	CA	PRO	219	2828	3120	4730	-410	379	-6	9	6
ATOM	1510	C	PRO	219	13.636	31.959	58.981	1.000	28.43			
ANISOU	1510	C	PRO	219	3141	3010	4653	-190	116	-3	2	8
ATOM	1511	O	PRO	219	12.904	32.393	58.081	1.000	34.17			
ANISOU	1511	O	PRO	219	4734	3500	4750	302	-798	-8	9	3
ATOM	1512	CB	PRO	219	13.115	32.717	61.316	1.000	39.70			
ANISOU	1512	CB	PRO	219	5621	3612	5852	-500	1615	-1	5	2
ATOM	1513	CG	PRO	219	13.368	32.033	62.628	1.000	42.38			
ANISOU	1513	CG	PRO	219	6139	5277	4688	-257	2084	-2	0	8
ATOM	1514	CD	PRO	219	14.370	30.943	62.289	1.000	32.77			
ANISOU	1514	CD	PRO	219	3901	5719	2831	-602	828	-1	6	0
ATOM	1515	N	ASP	220	14.950	31.824	58.811	1.000	25.65			
ANISOU	1515	N	ASP	220	3328	1582	4837	-276	801	-8	7	8
ATOM	1516	CA	ASP	220	15.590	32.280	57.587	1.000	26.45			
ANISOU	1516	CA	ASP	220	3594	2115	4341	-782	248	-8	6	1
ATOM	1517	C	ASP	220	15.781	31.305	56.451	1.000	28.46			
ANISOU	1517	C	ASP	220	3549	1843	5423	-111	1638	-9	4	3
ATOM	1518	O	ASP	220	16.432	31.620	55.433	1.000	25.80			
ANISOU	1518	O	ASP	220	3249	2021	4533	-140	623	-4	1	2
ATOM	1519	CB	ASP	220	16.911	32.962	57.998	1.000	33.76			
ANISOU	1519	CB	ASP	220	2351	3539	6938	-445	1187	-1	7	2
ATOM	1520	CG	ASP	220	17.882	31.913	58.502	1.000	42.36			
ANISOU	1520	CG	ASP	220	2653	3531	9912	-812	230	-9	5	7
ATOM	1521	OD1	ASP	220	17.484	31.170	59.423	1.000	37.00			
ANISOU	1521	OD1	ASP	220	3154	4148	6757	-104	-410	-2	0	0
ATOM	1522	OD2	ASP	220	18.981	31.787	57.957	1.000	37.34			
ANISOU	1522	OD2	ASP	220	2520	4700	6969	93	-824	-1	2	6
ATOM	1523	N	ALA	221	15.292	30.072	56.537	1.000	24.79			
ANISOU	1523	N	ALA	221	4148	1872	3398	-252	671	-6	5	9
ATOM	1524	CA	ALA	221	15.695	29.016	55.596	1.000	19.17			
ANISOU	1524	CA	ALA	221	2165	1868	3251	-52	-92	-6	1	0
ATOM	1525	C	ALA	221	14.551	27.996	55.479	1.000	18.60			
ANISOU	1525	C	ALA	221	1920	2238	2908	-82	-207	-3	6	2

-63-

ATOM	1526	O	ALA	221	13.763	27.852	56.415	1.000	26.47
ANISOU	1526	O	ALA	221	4127	2641	3289	-1307	894 -904
ATOM	1527	CB	ALA	221	16.939	28.316	56.104	1.000	19.36
ANISOU	1527	CB	ALA	221	2054	2333	2969	-537	-316 6 6
ATOM	1528	N	VAL	222	14.490	27.385	54.313	1.000	17.35
ANISOU	1528	N	VAL	222	2089	1841	2661	-101	-323 -154
ATOM	1529	CA	VAL	222	13.556	26.276	54.083	1.000	17.45
ANISOU	1529	CA	VAL	222	1620	2004	3004	-66	-417 1 9
ATOM	1530	C	VAL	222	14.333	24.965	54.077	1.000	15.69
ANISOU	1530	C	VAL	222	1616	1876	2471	-269	-349 -324
ATOM	1531	O	VAL	222	15.512	24.934	53.716	1.000	17.84
ANISOU	1531	O	VAL	222	1658	1730	3390	-108	-194 4 8
ATOM	1532	CB	VAL	222	12.822	26.433	52.747	1.000	19.60
ANISOU	1532	CB	VAL	222	2267	2202	2979	91 -666	-304
ATOM	1533	CG1	VAL	222	13.781	26.363	51.563	1.000	21.96
ANISOU	1533	CG1	VAL	222	2252	3113	2977	250	-645 -182
ATOM	1534	CG2	VAL	222	11.730	25.411	52.490	1.000	22.44
ANISOU	1534	CG2	VAL	222	2923	2537	3067	-497	-898 4 4
ATOM	1535	N	LEU	223	13.789	23.892	54.621	1.000	16.30
ANISOU	1535	N	LEU	223	1792	1694	2706	-239	-93 -532
ATOM	1536	CA	LEU	223	14.407	22.575	54.579	1.000	15.91
ANISOU	1536	CA	LEU	223	1679	1864	2503	-93	-297 -333
ATOM	1537	C	LEU	223	14.114	21.908	53.243	1.000	14.86
ANISOU	1537	C	LEU	223	1337	1537	2773	-141	-322 -458
ATOM	1538	O	LEU	223	12.969	21.888	52.766	1.000	16.23
ANISOU	1538	O	LEU	223	1317	2132	2719	70 -391	-281
ATOM	1539	CB	LEU	223	13.829	21.779	55.761	1.000	19.97
ANISOU	1539	CB	LEU	223	2740	1945	2901	-121	205 -212
ATOM	1540	CG	LEU	223	14.298	20.348	55.882	1.000	23.01
ANISOU	1540	CG	LEU	223	2668	1871	4205	-375	-170 9 1
ATOM	1541	CD1	LEU	223	15.797	20.322	56.143	1.000	23.73
ANISOU	1541	CD1	LEU	223	2570	3067	3378	69	135 3 16
ATOM	1542	CD2	LEU	223	13.492	19.668	56.979	1.000	35.71
ANISOU	1542	CD2	LEU	223	2813	3296	7459	525	1116 2333
ATOM	1543	N	VAL	224	15.115	21.370	52.570	1.000	14.18
ANISOU	1543	N	VAL	224	1383	1446	2560	-28	-320 -205
ATOM	1544	CA	VAL	224	14.956	20.627	51.330	1.000	14.52
ANISOU	1544	CA	VAL	224	1585	1501	2431	-23	-323 -127
ATOM	1545	C	VAL	224	15.320	19.160	51.561	1.000	13.59
ANISOU	1545	C	VAL	224	1464	1522	2178	23 -290	-251
ATOM	1546	O	VAL	224	16.442	18.861	51.981	1.000	15.38
ANISOU	1546	O	VAL	224	1464	1558	2822	0 -505	-374
ATOM	1547	CB	VAL	224	15.832	21.209	50.222	1.000	14.25
ANISOU	1547	CB	VAL	224	1402	1606	2407	-60	-461 -108
ATOM	1548	CG1	VAL	224	15.685	20.443	48.906	1.000	16.63
ANISOU	1548	CG1	VAL	224	1682	2164	2474	-159	-408 -421
ATOM	1549	CG2	VAL	224	15.575	22.687	50.040	1.000	16.40
ANISOU	1549	CG2	VAL	224	1807	1562	2863	6 -509	8 7
ATOM	1550	N	PHE	225	14.340	18.299	51.299	1.000	13.49
ANISOU	1550	N	PHE	225	1494	1526	2106	-66	-353 -130
ATOM	1551	CA	PHE	225	14.647	16.882	51.162	1.000	14.67
ANISOU	1551	CA	PHE	225	1639	1505	2431	-115	-61 -283
ATOM	1552	C	PHE	225	14.756	16.533	49.675	1.000	14.27
ANISOU	1552	C	PHE	225	1536	1533	2352	100	-260 -194
ATOM	1553	O	PHE	225	13.858	16.876	48.893	1.000	16.25
ANISOU	1553	O	PHE	225	1604	2000	2569	296	-311 -88
ATOM	1554	CB	PHE	225	13.537	15.999	51.749	1.000	15.57
ANISOU	1554	CB	PHE	225	1613	1563	2740	-25	-46 2 4
ATOM	1555	CG	PHE	225	13.387	15.996	53.257	1.000	17.95
ANISOU	1555	CG	PHE	225	1888	2267	2666	-650	-302 203
ATOM	1556	CD1	PHE	225	14.409	15.809	54.157	1.000	27.39

- 64 -

ANISOU	1556	CD1	PHE	225	2740	4234	3431	-910	-1094	9 0 0
ATOM	1557	CD2	PHE	225	12.125	15.863	53.820	1.000	21.09	
ANISOU	1557	CD2	PHE	225	2333	2765	2917	-166	399	- 5 2 7
ATOM	1558	CE1	PHE	225	14.211	15.673	55.521	1.000	26.82	
ANISOU	1558	CE1	PHE	225	3108	3657	3424	-1044	-1241	1 1 2 8
ATOM	1559	CE2	PHE	225	11.910	15.910	55.186	1.000	21.65	
ANISOU	1559	CE2	PHE	225	2994	2414	2817	623	239	- 3 9
ATOM	1560	CZ	PHE	225	12.958	15.787	56.078	1.000	28.82	
ANISOU	1560	CZ	PHE	225	3705	3716	3531	-832	-663	3 4 0
ATOM	1561	N	CYS	226	15.795	15.817	49.266	1.000	12.77	
ANISOU	1561	N	CYS	226	1428	1292	2131	-60	-370	- 2 3 9
ATOM	1562	CA	CYS	226	15.810	15.180	47.956	1.000	12.99	
ANISOU	1562	CA	CYS	226	1360	1440	2135	12	-355	- 2 0 7
ATOM	1563	C	CYS	226	14.903	13.956	47.985	1.000	12.37	
ANISOU	1563	C	CYS	226	1533	1212	1955	8	-283	- 3 1 1
ATOM	1564	O	CYS	226	14.961	13.217	48.974	1.000	15.68	
ANISOU	1564	O	CYS	226	1885	1651	2424	-140	-611	1 5 8
ATOM	1565	CB	CYS	226	17.228	14.855	47.527	1.000	13.77	
ANISOU	1565	CB	CYS	226	1410	1627	2193	19	-203	- 7 5
ATOM	1566	SG	CYS	226	18.224	16.367	47.314	1.000	16.37	
ANISOU	1566	SG	CYS	226	1744	1740	2735	-222	-236	- 1 2
ATOM	1567	N	GLY	227	14.150	13.722	46.928	1.000	13.20	
ANISOU	1567	N	GLY	227	1388	1513	2113	-28	-293	- 2 9 0
ATOM	1568	CA	GLY	227	13.352	12.496	46.899	1.000	12.58	
ANISOU	1568	CA	GLY	227	1279	1631	1872	-83	-438	- 2 5 5
ATOM	1569	C	GLY	227	13.903	11.541	45.849	1.000	12.54	
ANISOU	1569	C	GLY	227	1518	1279	1965	15	-288	- 7 9
ATOM	1570	O	GLY	227	14.917	11.732	45.152	1.000	13.58	
ANISOU	1570	O	GLY	227	1630	1523	2008	51	-155	8 2
ATOM	1571	N	ALA	228	13.212	10.400	45.712	1.000	13.02	
ANISOU	1571	N	ALA	228	1490	1306	2151	59	-204	- 1 6 1
ATOM	1572	CA	ALA	228	13.663	9.321	44.860	1.000	12.41	
ANISOU	1572	CA	ALA	228	1649	1155	1912	-68	-119	- 6 3
ATOM	1573	C	ALA	228	13.706	9.727	43.404	1.000	12.82	
ANISOU	1573	C	ALA	228	1566	1288	2016	97	-223	- 5
ATOM	1574	O	ALA	228	14.482	9.132	42.651	1.000	13.64	
ANISOU	1574	O	ALA	228	1717	1462	2004	26	-6	- 1 3 1
ATOM	1575	CB	ALA	228	12.714	8.121	45.058	1.000	14.56	
ANISOU	1575	CB	ALA	228	1808	1366	2356	-219	358	- 2 4 3
ATOM	1576	N	ILE	229	12.909	10.695	42.952	1.000	13.61	
ANISOU	1576	N	ILE	229	1340	1391	2441	-43	-289	2 7 3
ATOM	1577	CA	ILE	229	13.024	11.131	41.566	1.000	12.93	
ANISOU	1577	CA	ILE	229	1325	1243	2344	-42	-306	1 7 3
ATOM	1578	C	ILE	229	14.342	11.864	41.358	1.000	13.17	
ANISOU	1578	C	ILE	229	1327	1364	2311	-47	-191	1 3 0
ATOM	1579	O	ILE	229	14.938	11.746	40.262	1.000	14.41	
ANISOU	1579	O	ILE	229	1587	1596	2293	-37	-167	1 8 3
ATOM	1580	CB	ILE	229	11.768	11.888	41.103	1.000	13.46	
ANISOU	1580	CB	ILE	229	1470	1631	2015	171	-354	- 4 2
ATOM	1581	CG1	ILE	229	10.599	10.920	40.973	1.000	15.72	
ANISOU	1581	CG1	ILE	229	1218	1936	2817	85	31	1 1 8
ATOM	1582	CG2	ILE	229	12.040	12.674	39.808	1.000	14.19	
ANISOU	1582	CG2	ILE	229	1670	1425	2298	76	-364	1 7 4
ATOM	1583	CD1	ILE	229	10.745	9.924	39.836	1.000	20.03	
ANISOU	1583	CD1	ILE	229	2129	1814	3667	-208	-385	- 4 8 8
ATOM	1584	N	ALA	230	14.877	12.575	42.353	1.000	13.38	
ANISOU	1584	N	ALA	230	1252	1378	2454	-97	-176	7 4
ATOM	1585	CA	ALA	230	16.209	13.185	42.130	1.000	12.30	
ANISOU	1585	CA	ALA	230	1156	1444	2074	66	-97	- 1 0 8
ATOM	1586	C	ALA	230	17.223	12.033	41.976	1.000	12.89	
ANISOU	1586	C	ALA	230	1491	1327	2079	128	30	- 2 0

- 65 -

ATOM	1587	O	ALA	230	18.100	12.091	41.146	1.000	13.65
ANISOU	1587	O	ALA	230	1240	1530	2418	108	4 4 6
ATOM	1588	CB	ALA	230	16.588	14.000	43.345	1.000	13.66
ANISOU	1588	CB	ALA	230	1559	1415	2215	-186	-21 - 2 2 9
ATOM	1589	N	THR	231	17.143	10.978	42.805	1.000	13.31
ANISOU	1589	N	THR	231	1526	1318	2214	58	-261 - 1
ATOM	1590	CA	THR	231	18.022	9.815	42.659	1.000	13.32
ANISOU	1590	CA	THR	231	1660	1307	2093	78	-302 3 2
ATOM	1591	C	THR	231	17.906	9.224	41.251	1.000	13.27
ANISOU	1591	C	THR	231	1300	1631	2111	205	-211 3
ATOM	1592	O	THR	231	18.932	8.974	40.620	1.000	15.51
ANISOU	1592	O	THR	231	1468	1759	2667	245	58 - 1 7 0
ATOM	1593	CB	THR	231	17.656	8.751	43.688	1.000	13.03
ANISOU	1593	CB	THR	231	1500	1302	2151	46	-166 1 2
ATOM	1594	OG1	THR	231	17.530	9.313	44.995	1.000	14.70
ANISOU	1594	OG1	THR	231	1742	1614	2230	-99	32 - 1 4
ATOM	1595	CG2	THR	231	18.698	7.621	43.697	1.000	13.69
ANISOU	1595	CG2	THR	231	1449	1419	2335	113	-211 1 9 7
ATOM	1596	N	LEU	232	16.665	9.049	40.796	1.000	13.43
ANISOU	1596	N	LEU	232	1447	1384	2271	75	-404 - 2 7
ATOM	1597	CA	LEU	232	16.446	8.396	39.527	1.000	14.11
ANISOU	1597	CA	LEU	232	1809	1226	2326	80	-468 4 9
ATOM	1598	C	LEU	232	16.975	9.248	38.381	1.000	15.53
ANISOU	1598	C	LEU	232	1968	1557	2376	209	-3 9 0
ATOM	1599	O	LEU	232	17.749	8.808	37.504	1.000	17.16
ANISOU	1599	O	LEU	232	2024	1949	2546	107	-116 - 5 1 9
ATOM	1600	CB	LEU	232	14.940	8.135	39.368	1.000	14.47
ANISOU	1600	CB	LEU	232	1692	1630	2175	72	-396 - 1 6 1
ATOM	1601	CG	LEU	232	14.525	7.307	38.155	1.000	15.89
ANISOU	1601	CG	LEU	232	1941	1768	2329	120	-470 - 3 0 3
ATOM	1602	CD1	LEU	232	15.118	5.920	38.202	1.000	23.19
ANISOU	1602	CD1	LEU	232	3565	2020	3228	743	-1110 - 8 5 1
ATOM	1603	CD2	LEU	232	13.003	7.190	38.126	1.000	19.46
ANISOU	1603	CD2	LEU	232	2006	2262	3126	-470	-523 - 6 6
ATOM	1604	N	VAL	233	16.539	10.514	38.299	1.000	13.73
ANISOU	1604	N	VAL	233	1736	1454	2025	-7	-263 1 9 3
ATOM	1605	CA	VAL	233	16.893	11.317	37.117	1.000	13.84
ANISOU	1605	CA	VAL	233	1674	1658	1926	141	-73 1 0 7
ATOM	1606	C	VAL	233	18.407	11.510	37.025	1.000	14.08
ANISOU	1606	C	VAL	233	1716	1674	1958	72	-46 1 1 3
ATOM	1607	O	VAL	233	18.940	11.587	35.910	1.000	16.65
ANISOU	1607	O	VAL	233	1923	2325	2079	38	109 4 0 1
ATOM	1608	CB	VAL	233	16.098	12.626	37.062	1.000	14.69
ANISOU	1608	CB	VAL	233	1680	1696	2206	141	-165 3 3 3
ATOM	1609	CG1	VAL	233	16.529	13.650	38.113	1.000	15.70
ANISOU	1609	CG1	VAL	233	1615	1654	2698	34	156 - 2 8
ATOM	1610	CG2	VAL	233	16.117	13.206	35.647	1.000	16.43
ANISOU	1610	CG2	VAL	233	1740	2041	2459	251	117 5 9 6
ATOM	1611	N	THR	234	19.100	11.594	38.175	1.000	14.23
ANISOU	1611	N	THR	234	1599	1724	2083	146	-110 2 3 5
ATOM	1612	CA	THR	234	20.524	11.908	38.148	1.000	16.14
ANISOU	1612	CA	THR	234	1664	1868	2602	63	-171 - 4 9
ATOM	1613	C	THR	234	21.346	10.621	38.006	1.000	17.09
ANISOU	1613	C	THR	234	1717	1865	2912	146	211 - 5 1
ATOM	1614	O	THR	234	22.558	10.644	38.139	1.000	17.25
ANISOU	1614	O	THR	234	1776	1951	2828	108	200 2 2 9
ATOM	1615	CB	THR	234	21.030	12.681	39.373	1.000	15.29
ANISOU	1615	CB	THR	234	1667	1502	2642	-46	-149 1 6 3
ATOM	1616	OG1	THR	234	20.849	11.819	40.522	1.000	15.45
ANISOU	1616	OG1	THR	234	1659	1708	2502	-80	59 4 4
ATOM	1617	CG2	THR	234	20.291	13.978	39.597	1.000	16.61

- 66 -

ANISOU	1617	CG2	THR	234	1564	1672	3077	3	-34	-4	2
ATOM	1618	N	GLY	235	20.712	9.441	37.833	1.000	16	80	
ANISOU	1618	N	GLY	235	1905	1914	2564	193	29	-2	19
ATOM	1619	CA	GLY	235	21.484	8.209	37.792	1.000	17	10	
ANISOU	1619	CA	GLY	235	2049	1861	2586	133	223	-4	88
ATOM	1620	C	GLY	235	22.225	7.931	39.083	1.000	18	06	
ANISOU	1620	C	GLY	235	2046	2049	2768	419	499	3	03
ATOM	1621	O	GLY	235	23.285	7.289	39.010	1.000	21	26	
ANISOU	1621	O	GLY	235	2167	2606	3303	679	343	-7	4
ATOM	1622	N	GLY	236	21.602	8.149	40.237	1.000	16	17	
ANISOU	1622	N	GLY	236	1663	1901	2582	36	291	3	05
ATOM	1623	CA	GLY	236	22.080	7.673	41.520	1.000	17	27	
ANISOU	1623	CA	GLY	236	2135	1671	2754	225	28	2	29
ATOM	1624	C	GLY	236	23.033	8.639	42.194	1.000	16	88	
ANISOU	1624	C	GLY	236	1880	1890	2644	204	100	2	22
ATOM	1625	O	GLY	236	23.692	8.272	43.193	1.000	19	42	
ANISOU	1625	O	GLY	236	2165	2399	2814	314	-90	4	19
ATOM	1626	N	GLN	237	23.134	9.890	41.746	1.000	16	99	
ANISOU	1626	N	GLN	237	1647	1851	2957	213	-213	1	67
ATOM	1627	CA	GLN	237	24.074	10.849	42.298	1.000	16	75	
ANISOU	1627	CA	GLN	237	1608	2004	2752	72	177	9	8
ATOM	1628	C	GLN	237	23.481	11.604	43.483	1.000	15	64	
ANISOU	1628	C	GLN	237	1404	2136	2402	231	-146	2	00
ATOM	1629	O	GLN	237	24.183	12.382	44.164	1.000	18	17	
ANISOU	1629	O	GLN	237	1581	2508	2817	-227	-6	-4	6
ATOM	1630	CB	GLN	237	24.456	11.855	41.217	1.000	17	17	
ANISOU	1630	CB	GLN	237	1912	2080	2532	71	141	-7	
ATOM	1631	CG	GLN	237	25.304	11.221	40.115	1.000	17	64	
ANISOU	1631	CG	GLN	237	1850	2410	2441	226	95	-3	0
ATOM	1632	CD	GLN	237	25.721	12.302	39.137	1.000	19	72	
ANISOU	1632	CD	GLN	237	1680	2833	2979	104	317	3	07
ATOM	1633	OE1	GLN	237	26.602	13.110	39.436	1.000	24	27	
ANISOU	1633	OE1	GLN	237	1841	3145	4234	-213	-187	8	09
ATOM	1634	NE2	GLN	237	24.986	12.399	38.027	1.000	18	53	
ANISOU	1634	NE2	GLN	237	2007	2298	2735	432	374	2	02
ATOM	1635	N	VAL	238	22.221	11.359	43.807	1.000	14	75	
ANISOU	1635	N	VAL	238	1563	1804	2237	-32	-54	4	3
ATOM	1636	CA	VAL	238	21.533	12.075	44.862	1.000	14	41	
ANISOU	1636	CA	VAL	238	1535	1553	2388	0	-44	3	2
ATOM	1637	C	VAL	238	20.861	11.060	45.781	1.000	13	56	
ANISOU	1637	C	VAL	238	1414	1392	2346	82	55	-1	49
ATOM	1638	O	VAL	238	20.136	10.174	45.302	1.000	15	87	
ANISOU	1638	O	VAL	238	1655	1639	2737	-218	-285	-2	2
ATOM	1639	CB	VAL	238	20.467	13.061	44.309	1.000	14	73	
ANISOU	1639	CB	VAL	238	1817	1626	2152	35	-437	-9	5
ATOM	1640	CG1	VAL	238	19.805	13.764	45.489	1.000	15	70	
ANISOU	1640	CG1	VAL	238	1965	1490	2510	174	-524	-4	23
ATOM	1641	CG2	VAL	238	21.064	13.994	43.280	1.000	16	82	
ANISOU	1641	CG2	VAL	238	1862	1718	2812	-60	-378	2	22
ATOM	1642	N	LYS	239	21.119	11.153	47.071	1.000	14	47	
ANISOU	1642	N	LYS	239	1704	1474	2318	14	-40	1	2
ATOM	1643	CA	LYS	239	20.470	10.360	48.104	1.000	14	43	
ANISOU	1643	CA	LYS	239	1460	1617	2406	106	-168	1	79
ATOM	1644	C	LYS	239	19.048	10.852	48.409	1.000	14	82	
ANISOU	1644	C	LYS	239	1533	1456	2642	102	-53	2	32
ATOM	1645	O	LYS	239	18.839	12.067	48.457	1.000	14	74	
ANISOU	1645	O	LYS	239	1841	1442	2318	158	-275	1	90
ATOM	1646	CB	LYS	239	21.320	10.435	49.385	1.000	16	40	
ANISOU	1646	CB	LYS	239	1995	1712	2527	243	-543	2	52
ATOM	1647	CG	LYS	239	20.767	9.549	50.498	1.000	16	65	
ANISOU	1647	CG	LYS	239	1954	1759	2614	-58	-781	2	44

- 67 -

ATOM	1648	CD	LYS	239	21.738	9.511	51.683	1.000	19.76	
ANISOU	1648	CD	LYS	239	2954	1820	2732	-123	-1234	3 6 3
ATOM	1649	CE	LYS	239	21.107	8.835	52.896	1.000	22.58	
ANISOU	1649	CE	LYS	239	3331	2164	3086	-652	-1502	8 6 3
ATOM	1650	NZ	LYS	239	21.904	8.883	54.145	1.000	23.13	
ANISOU	1650	NZ	LYS	239	2817	3360	2612	-471	-943	2 8 7
ATOM	1651	N	ALA	240	18.140	9.892	48.659	1.000	14.35	
ANISOU	1651	N	ALA	240	1429	1607	2418	-156	-334	- 6 1
ATOM	1652	CA	ALA	240	16.791	10.192	49.145	1.000	13.98	
ANISOU	1652	CA	ALA	240	1468	1635	2210	-151	-335	- 1 0
ATOM	1653	C	ALA	240	16.728	9.776	50.605	1.000	13.44	
ANISOU	1653	C	ALA	240	1439	1388	2279	77	-450	2 2
ATOM	1654	O	ALA	240	16.514	8.592	50.913	1.000	16.32	
ANISOU	1654	O	ALA	240	1932	1567	2699	-215	-673	3 1 4
ATOM	1655	CB	ALA	240	15.712	9.565	48.268	1.000	15.21	
ANISOU	1655	CB	ALA	240	1510	1962	2306	-104	-387	- 3 0 7
ATOM	1656	N	PRO	241	16.907	10.701	51.546	1.000	14.23	
ANISOU	1656	N	PRO	241	1634	1551	2221	-87	-292	7 1
ATOM	1657	CA	PRO	241	17.035	10.251	52.940	1.000	14.68	
ANISOU	1657	CA	PRO	241	1718	1681	2180	-350	-174	- 3 0
ATOM	1658	C	PRO	241	15.693	9.961	53.579	1.000	13.89	
ANISOU	1658	C	PRO	241	1659	1581	2039	-107	-207	- 7 4
ATOM	1659	O	PRO	241	14.629	10.527	53.261	1.000	17.06	
ANISOU	1659	O	PRO	241	1698	1946	2838	17	-254	1 4 6
ATOM	1660	CB	PRO	241	17.689	11.462	53.619	1.000	16.63	
ANISOU	1660	CB	PRO	241	2162	1657	2501	-460	-487	5 5
ATOM	1661	CG	PRO	241	17.138	12.651	52.826	1.000	16.56	
ANISOU	1661	CG	PRO	241	2433	1601	2258	-367	-274	3 1
ATOM	1662	CD	PRO	241	17.164	12.140	51.409	1.000	14.92	
ANISOU	1662	CD	PRO	241	1841	1490	2339	-215	-186	- 6 6
ATOM	1663	N	ARG	242	15.740	9.049	54.544	1.000	15.74	
ANISOU	1663	N	ARG	242	1914	1853	2212	-381	-308	2 0 4
ATOM	1664	CA	ARG	242	14.574	8.772	55.376	1.000	15.50	
ANISOU	1664	CA	ARG	242	1955	1863	2073	-236	-291	1 8 0
ATOM	1665	C	ARG	242	14.406	9.841	56.437	1.000	16.60	
ANISOU	1665	C	ARG	242	1889	2011	2407	-120	-411	- 5 1
ATOM	1666	O	ARG	242	15.372	10.416	56.994	1.000	18.31	
ANISOU	1666	O	ARG	242	2041	2186	2732	-216	-559	- 1 8 0
ATOM	1667	CB	ARG	242	14.728	7.419	56.085	1.000	18.38	
ANISOU	1667	CB	ARG	242	2920	1810	2253	-486	-391	2 6 9
ATOM	1668	CG	ARG	242	14.564	6.273	55.094	1.000	18.42	
ANISOU	1668	CG	ARG	242	2372	1873	2755	-88	162	- 1 5 5
ATOM	1669	CD	ARG	242	14.854	4.935	55.796	1.000	23.07	
ANISOU	1669	CD	ARG	242	3380	2022	3366	470	-483	- 2 1 7
ATOM	1670	NE	ARG	242	16.334	4.954	55.991	1.000	26.69	
ANISOU	1670	NE	ARG	242	3498	2727	3916	444	-829	4 7
ATOM	1671	CZ	ARG	242	16.941	3.921	56.584	1.000	27.19	
ANISOU	1671	CZ	ARG	242	3166	2879	4284	-297	-1143	8 0 2
ATOM	1672	NH1	ARG	242	16.157	2.913	56.989	1.000	33.14	
ANISOU	1672	NH1	ARG	242	3810	3235	5546	-316	528	7 2 6
ATOM	1673	NH2	ARG	242	18.241	3.889	56.779	1.000	31.13	
ANISOU	1673	NH2	ARG	242	3043	2925	5859	227	-769	4 8 4
ATOM	1674	N	HIS	243	13.188	10.057	56.872	1.000	17.55	
ANISOU	1674	N	HIS	243	1979	2233	2457	-165	-173	- 7 4
ATOM	1675	CA	HIS	243	12.913	11.050	57.914	1.000	17.84	
ANISOU	1675	CA	HIS	243	2186	2139	2452	-260	-123	- 7 5
ATOM	1676	C	HIS	243	11.644	10.627	58.643	1.000	17.52	
ANISOU	1676	C	HIS	243	2102	2084	2470	-248	-164	- 3 2 5
ATOM	1677	O	HIS	243	10.870	9.803	58.132	1.000	20.23	
ANISOU	1677	O	HIS	243	2226	2593	2868	-551	-323	- 3 9 2
ATOM	1678	CB	HIS	243	12.865	12.456	57.324	1.000	19.74	

- 68 -

ANISOU	1678	CB	HIS	243	2770	2248	2482	-188	-106	8	3
ATOM	1679	CG	HIS	243	11.922	12.630	56.187	1.000	22.60		
ANISOU	1679	CG	HIS	243	3449	2513	2624	164	-382	0	
ATOM	1680	ND1	HIS	243	12.209	12.299	54.879	1.000	25.87		
ANISOU	1680	ND1	HIS	243	4780	2575	2473	-609	-403	5	3
ATOM	1681	CD2	HIS	243	10.633	13.034	56.172	1.000	29.11		
ANISOU	1681	CD2	HIS	243	3220	4490	3348	121	-421	1	63 0
ATOM	1682	CE1	HIS	243	11.182	12.573	54.109	1.000	32.92		
ANISOU	1682	CE1	HIS	243	5835	3672	3001	-1102	-1367	6	8 9
ATOM	1683	NE2	HIS	243	10.214	13.012	54.875	1.000	36.95		
ANISOU	1683	NE2	HIS	243	5719	4201	4119	1019	-2016	9	8 7
ATOM	1684	N	HIS	244	11.437	11.194	59.831	1.000	18.87		
ANISOU	1684	N	HIS	244	2523	2477	2171	-88	-141	-1	1 7
ATOM	1685	CA	HIS	244	10.302	10.801	60.649	1.000	20.83		
ANISOU	1685	CA	HIS	244	2802	2485	2628	171	251	2	7 2
ATOM	1686	C	HIS	244	9.927	11.968	61.551	1.000	20.33		
ANISOU	1686	C	HIS	244	1803	2969	2953	-31	-78	-2	7 3
ATOM	1687	O	HIS	244	10.482	13.073	61.510	1.000	21.71		
ANISOU	1687	O	HIS	244	2057	3418	2774	-535	145	-8	5 3
ATOM	1688	CB	HIS	244	10.714	9.557	61.468	1.000	24.38		
ANISOU	1688	CB	HIS	244	4066	2644	2553	-76	-390	4	4 1
ATOM	1689	CG	HIS	244	11.859	9.725	62.423	1.000	28.34		
ANISOU	1689	CG	HIS	244	4158	3498	3113	696	-727	-8	9
ATOM	1690	ND1	HIS	244	13.132	9.205	62.268	1.000	32.35		
ANISOU	1690	ND1	HIS	244	4012	4471	3808	548	-485	-8	5 0
ATOM	1691	CD2	HIS	244	11.928	10.391	63.609	1.000	25.21		
ANISOU	1691	CD2	HIS	244	2937	4137	2505	-373	45	2	1 9
ATOM	1692	CE1	HIS	244	13.887	9.531	63.312	1.000	31.71		
ANISOU	1692	CE1	HIS	244	4157	4277	3613	1224	-749	-5	1 8
ATOM	1693	NE2	HIS	244	13.146	10.263	64.150	1.000	24.52		
ANISOU	1693	NE2	HIS	244	3165	3517	2633	94	-82	4	9 2
ATOM	1694	N	VAL	245	8.890	11.687	62.349	1.000	23.87		
ANISOU	1694	N	VAL	245	2627	3119	3322	-251	531	-3	1 0
ATOM	1695	CA	VAL	245	8.473	12.691	63.349	1.000	24.85		
ANISOU	1695	CA	VAL	245	2785	3770	2888	481	149	-2	9 3
ATOM	1696	C	VAL	245	8.624	12.079	64.735	1.000	26.03		
ANISOU	1696	C	VAL	245	3220	3558	3112	-289	179	8	9
ATOM	1697	O	VAL	245	8.023	11.025	64.969	1.000	27.98		
ANISOU	1697	O	VAL	245	3120	3085	4428	42	295	-5	9
ATOM	1698	CB	VAL	245	7.020	13.114	63.099	1.000	26.02		
ANISOU	1698	CB	VAL	245	2621	3489	3777	94	-103	-5	6 9
ATOM	1699	CG1	VAL	245	6.586	14.114	64.161	1.000	28.06		
ANISOU	1699	CG1	VAL	245	2717	3330	4614	159	746	-4	8 5
ATOM	1700	CG2	VAL	245	6.927	13.705	61.680	1.000	30.51		
ANISOU	1700	CG2	VAL	245	3564	3809	4220	1264	-305	-3	3
ATOM	1701	N	ALA	246	9.399	12.696	65.603	1.000	28.08		
ANISOU	1701	N	ALA	246	4338	3787	2543	-850	250	2	5 4
ATOM	1702	CA	ALA	246	9.567	12.316	67.003	1.000	27.45		
ANISOU	1702	CA	ALA	246	4363	3360	2707	292	275	3	7 3
ATOM	1703	C	ALA	246	8.356	12.740	67.833	1.000	32.68		
ANISOU	1703	C	ALA	246	4915	4473	3031	98	880	1	9 7
ATOM	1704	O	ALA	246	7.774	13.791	67.563	1.000	29.54		
ANISOU	1704	O	ALA	246	3522	4283	3417	-224	875	-3	2 9
ATOM	1705	CB	ALA	246	10.819	13.010	67.542	1.000	30.33		
ANISOU	1705	CB	ALA	246	4564	3949	3011	615	-221	-4	2 2
ATOM	1706	N	ALA	247	8.048	11.958	68.849	1.000	34.09		
ANISOU	1706	N	ALA	247	4483	5156	3311	-1190	466	3	9 3
ATOM	1707	CA	ALA	247	7.036	12.190	69.859	1.000	34.23		
ANISOU	1707	CA	ALA	247	4188	5627	3189	-1215	315	5	1 5
ATOM	1708	C	ALA	247	7.609	12.910	71.081	1.000	33.31		
ANISOU	1708	C	ALA	247	5419	4684	2555	249	-506	1	1 4 7

- 69 -

ATOM 1709 O ALA 247 8.733 12.708 71.523 1.000 38.23
 ANISOU 1709 O ALA 247 5787 4478 4259 -378 -1519 1 2 3 0
 ATOM 1710 CB ALA 247 6.383 10.881 70.314 1.000 47.11
 ANISOU 1710 CB ALA 247 8374 6726 2801 -2800 1464 6 8 6
 ATOM 1711 N PRO 248 6.817 13.851 71.577 1.000 42.28
 ANISOU 1711 N PRO 248 5771 5458 4836 -300 933 -9 7
 ATOM 1712 CA PRO 248 7.256 14.581 72.773 1.000 44.85
 ANISOU 1712 CA PRO 248 7568 5478 3996 -645 1413 2 1 4
 ATOM 1713 C PRO 248 7.161 13.618 73.948 1.000 49.25
 ANISOU 1713 C PRO 248 7978 5660 5075 -1446 552 9 8 5
 ATOM 1714 O PRO 248 6.251 12.794 74.014 1.000 45.48
 ANISOU 1714 O PRO 248 7651 5391 4237 -1127 2573 -7 9 6
 ATOM 1715 CB PRO 248 6.196 15.674 72.897 1.000 49.75
 ANISOU 1715 CB PRO 248 8563 4816 5523 -513 1238 -1 3 8
 ATOM 1716 CG PRO 248 4.973 15.053 72.299 1.000 50.89
 ANISOU 1716 CG PRO 248 7228 5564 6545 -108 2210 -1 0 6 4
 ATOM 1717 CD PRO 248 5.489 14.272 71.114 1.000 44.69
 ANISOU 1717 CD PRO 248 6395 4579 6006 937 953 -5 7 7
 ATOM 1718 N ARG 249 8.109 13.683 74.883 1.000 48.76
 ANISOU 1718 N ARG 249 9141 6341 3045 -1317 1069 -4 7 7
 ATOM 1719 CA ARG 249 7.865 12.783 76.024 1.000 55.51
 ANISOU 1719 CA ARG 249 10023 6914 4156 -1098 895 5 6 6
 ATOM 1720 C ARG 249 6.844 13.466 76.916 1.000 46.09
 ANISOU 1720 C ARG 249 5561 8382 3568 -2484 -7 1 2 3 7
 ATOM 1721 O ARG 249 6.244 12.915 77.831 1.000 56.25
 ANISOU 1721 O ARG 249 7572 6368 7433 -377 1799 3 9 9 5
 ATOM 1722 CB ARG 249 9.177 12.459 76.721 1.000 55.24
 ANISOU 1722 CB ARG 249 8950 7715 4326 705 2864 1 2 7 0
 ATOM 1723 CG ARG 249 9.915 11.278 76.110 1.000 71.04
 ANISOU 1723 CG ARG 249 12881 7330 6779 1135 3707 6 2 2
 ATOM 1724 CD ARG 249 10.403 10.303 77.165 1.000 72.89
 ANISOU 1724 CD ARG 249 11721 7991 7984 2171 2723 4 0 9
 ATOM 1725 NE ARG 249 11.124 9.162 76.580 1.000 70.73
 ANISOU 1725 NE ARG 249 8627 9977 8271 2362 2650 -2 6 6
 ATOM 1726 CZ ARG 249 12.039 8.493 77.282 1.000 72.71
 ANISOU 1726 CZ ARG 249 10269 9417 7942 2304 2153 1 3 3
 ATOM 1727 NH1 ARG 249 12.297 8.893 78.521 1.000 89.50
 ANISOU 1727 NH1 ARG 249 22286 6161 5559 2015 1622 3 8 7 4
 ATOM 1728 NH2 ARG 249 12.682 7.462 76.761 1.000 67.68
 ANISOU 1728 NH2 ARG 249 5358 10062 10295 1004 3886 2 2 1
 ATOM 1729 N ALA 254 1.981 18.918 75.430 1.000 85.24
 ANISOU 1729 N ALA 254 15501 7922 8964 -4581 -1437 2 3 4 7
 ATOM 1730 CA ALA 254 2.287 20.081 76.257 1.000 76.08
 ANISOU 1730 CA ALA 254 12510 8110 8286 -3993 1617 1 5 9 2
 ATOM 1731 C ALA 254 2.943 21.216 75.489 1.000 60.91
 ANISOU 1731 C ALA 254 8383 5719 9040 -506 2886 1 3 1 2
 ATOM 1732 O ALA 254 4.174 21.309 75.487 1.000 72.37
 ANISOU 1732 O ALA 254 8056 8109 11332 1602 4553 3 3 8 1
 ATOM 1733 CB ALA 254 3.264 19.667 77.351 1.000 60.48
 ANISOU 1733 CB ALA 254 12589 7262 3131 -866 4570 -1 1 1 2
 ATOM 1734 N GLY 255 2.200 22.108 74.846 1.000 54.40
 ANISOU 1734 N GLY 255 8029 5451 7190 594 2922 -9 4 0
 ATOM 1735 CA GLY 255 2.880 23.171 74.098 1.000 40.05
 ANISOU 1735 CA GLY 255 5181 4570 5465 1424 836 -9 2 1
 ATOM 1736 C GLY 255 3.640 22.565 72.921 1.000 38.82
 ANISOU 1736 C GLY 255 4227 4772 5749 557 702 -1 5 6 1
 ATOM 1737 O GLY 255 4.580 23.163 72.398 1.000 39.96
 ANISOU 1737 O GLY 255 2978 6491 5715 -128 -136 -2 2 2 6
 ATOM 1738 N SER 256 3.164 21.387 72.509 1.000 37.29
 ANISOU 1738 N SER 256 5047 4594 4527 389 11 -8 5 3
 ATOM 1739 CA SER 256 3.738 20.606 71.429 1.000 35.71

- 70 -

ANISOU	1739	CA	SER	256	4737	4533	4299	560	-501	-919
ATOM	1740	C	SER	256	2.983	20.742	70.118	1.000	34.93	
ANISOU	1740	C	SER	256	4584	4669	4019	-98	-85	9 1
ATOM	1741	O	SER	256	3.251	20.000	69.162	1.000	33.92	
ANISOU	1741	O	SER	256	3575	6107	3207	503	304	3 7 7
ATOM	1742	CB	SER	256	3.845	19.136	71.853	1.000	30.17	
ANISOU	1742	CB	SER	256	3125	4830	3509	624	212	-492
ATOM	1743	OG	SER	256	2.688	18.752	72.601	1.000	61.15	
ANISOU	1743	OG	SER	256	2987	8497	11750	451	1943	2 6 3 0
ATOM	1744	N	SER	257	2.065	21.700	70.030	1.000	35.54	
ANISOU	1744	N	SER	257	4037	5989	3479	347	242	-86
ATOM	1745	CA	SER	257	1.379	21.993	68.767	1.000	30.95	
ANISOU	1745	CA	SER	257	2824	5827	3109	170	672	-509
ATOM	1746	C	SER	257	2.378	22.538	67.760	1.000	30.63	
ANISOU	1746	C	SER	257	3181	5524	2934	-476	765	-1297
ATOM	1747	O	SER	257	3.359	23.159	68.199	1.000	34.70	
ANISOU	1747	O	SER	257	3500	6070	3616	-829	603	-1516
ATOM	1748	CB	SER	257	0.331	23.088	69.036	1.000	38.70	
ANISOU	1748	CB	SER	257	3085	6518	5103	796	1381	4 3 5
ATOM	1749	OG	SER	257	0.801	24.361	68.601	1.000	65.12	
ANISOU	1749	OG	SER	257	8002	5175	11565	-999	-3375	3 8 3
ATOM	1750	N	ARG	258	2.119	22.384	66.471	1.000	30.51	
ANISOU	1750	N	ARG	258	3668	5068	2855	-332	677	-995
ATOM	1751	CA	ARG	258	2.997	22.819	65.396	1.000	28.15	
ANISOU	1751	CA	ARG	258	3100	4620	2976	-106	358	-544
ATOM	1752	C	ARG	258	2.198	22.913	64.096	1.000	25.64	
ANISOU	1752	C	ARG	258	3488	3381	2872	-676	273	-904
ATOM	1753	O	ARG	258	1.132	22.294	63.981	1.000	24.93	
ANISOU	1753	O	ARG	258	3162	3240	3070	-441	478	-560
ATOM	1754	CB	ARG	258	4.175	21.873	65.154	1.000	27.21	
ANISOU	1754	CB	ARG	258	3158	4041	3141	-446	313	-1352
ATOM	1755	CG	ARG	258	3.861	20.508	64.570	1.000	30.90	
ANISOU	1755	CG	ARG	258	4782	3429	3531	-737	-738	-389
ATOM	1756	CD	ARG	258	5.039	19.537	64.769	1.000	36.65	
ANISOU	1756	CD	ARG	258	5937	3466	4523	106	477	3 0 6
ATOM	1757	NE	ARG	258	4.597	18.176	64.411	1.000	32.42	
ANISOU	1757	NE	ARG	258	3372	3858	5089	-85	-274	5 2 8
ATOM	1758	CZ	ARG	258	4.633	17.777	63.143	1.000	37.32	
ANISOU	1758	CZ	ARG	258	5670	2958	5553	155	680	4 3
ATOM	1759	NH1	ARG	258	5.075	18.622	62.217	1.000	29.98	
ANISOU	1759	NH1	ARG	258	3077	3435	4881	-150	-211	-103
ATOM	1760	NH2	ARG	258	4.210	16.566	62.824	1.000	38.66	
ANISOU	1760	NH2	ARG	258	5812	3151	5724	-190	-1632	8 6 5
ATOM	1761	N	THR	259	2.806	23.572	63.120	1.000	23.62	
ANISOU	1761	N	THR	259	2625	3578	2771	-519	315	-1037
ATOM	1762	CA	THR	259	2.337	23.482	61.730	1.000	21.97	
ANISOU	1762	CA	THR	259	2614	2934	2800	-36	247	-1041
ATOM	1763	C	THR	259	3.528	23.197	60.808	1.000	19.76	
ANISOU	1763	C	THR	259	2257	2663	2587	-38	21	-699
ATOM	1764	O	THR	259	4.698	23.411	61.159	1.000	21.13	
ANISOU	1764	O	THR	259	2464	3096	2468	-495	-10	-286
ATOM	1765	CB	THR	259	1.682	24.793	61.278	1.000	24.04	
ANISOU	1765	CB	THR	259	2125	3084	3927	70	-157	-1229
ATOM	1766	OG1	THR	259	2.697	25.790	61.041	1.000	23.14	
ANISOU	1766	OG1	THR	259	2297	2848	3648	196	-142	-829
ATOM	1767	CG2	THR	259	0.760	25.408	62.331	1.000	25.17	
ANISOU	1767	CG2	THR	259	2941	3229	3393	726	264	-136
ATOM	1768	N	SER	260	3.234	22.706	59.600	1.000	20.41	
ANISOU	1768	N	SER	260	2386	2762	2609	-61	74	-806
ATOM	1769	CA	SER	260	4.225	22.515	58.551	1.000	19.33	
ANISOU	1769	CA	SER	260	2488	2459	2399	192	8	-344

- 71 -

ATOM	1770	C	SER	260	3.587	22.871	57.210	1.000	18.78	
ANISOU	1770	C	SER	260	1996	2544	2595	-379	-264	-3 1 1
ATOM	1771	O	SER	260	2.375	22.758	56.988	1.000	21.20	
ANISOU	1771	O	SER	260	1917	2448	3689	-75	-269	-5 7 3
ATOM	1772	CB	SER	260	4.738	21.076	58.480	1.000	20.28	
ANISOU	1772	CB	SER	260	2491	2458	2755	160	-101	-4 9 5
ATOM	1773	OG	SER	260	3.656	20.197	58.227	1.000	22.70	
ANISOU	1773	OG	SER	260	2758	2574	3294	-113	-284	-1 6 9
ATOM	1774	N	SER	261	4.474	23.329	56.330	1.000	18.79	
ANISOU	1774	N	SER	261	2189	2215	2737	-55	-92	3 5
ATOM	1775	CA	SER	261	4.148	23.585	54.929	1.000	16.88	
ANISOU	1775	CA	SER	261	2074	1718	2622	22	-117	-4 0 4
ATOM	1776	C	SER	261	5.066	22.672	54.106	1.000	17.25	
ANISOU	1776	C	SER	261	1720	1833	3000	101	-350	-4 9 1
ATOM	1777	O	SER	261	6.272	22.876	54.173	1.000	19.96	
ANISOU	1777	O	SER	261	1712	2417	3456	50	-483	-7 8 1
ATOM	1778	CB	SER	261	4.471	25.028	54.503	1.000	19.95	
ANISOU	1778	CB	SER	261	2903	1675	3002	164	-113	-1 3 5
ATOM	1779	OG	SER	261	4.404	25.127	53.107	1.000	35.64	
ANISOU	1779	OG	SER	261	5435	4814	3293	-1089	-766	1 2 6 3
ATOM	1780	N	VAL	262	4.467	21.722	53.435	1.000	15.56	
ANISOU	1780	N	VAL	262	1751	2021	2140	-75	-40	-4 3 6
ATOM	1781	CA	VAL	262	5.247	20.713	52.711	1.000	15.41	
ANISOU	1781	CA	VAL	262	1871	1938	2048	43	21	-1 9 6
ATOM	1782	C	VAL	262	4.914	20.874	51.242	1.000	14.05	
ANISOU	1782	C	VAL	262	1460	1784	2095	-13	29	-1 4 4
ATOM	1783	O	VAL	262	3.759	20.712	50.844	1.000	15.45	
ANISOU	1783	O	VAL	262	1488	1900	2481	-175	-94	-1 9 1
ATOM	1784	CB	VAL	262	4.902	19.307	53.253	1.000	16.87	
ANISOU	1784	CB	VAL	262	2144	2005	2260	165	-164	2 3
ATOM	1785	CG1	VAL	262	5.567	18.275	52.364	1.000	20.01	
ANISOU	1785	CG1	VAL	262	2433	2006	3165	4	-191	-6 3 7
ATOM	1786	CG2	VAL	262	5.335	19.200	54.715	1.000	18.63	
ANISOU	1786	CG2	VAL	262	2390	2242	2446	147	-397	1 7 5
ATOM	1787	N	PHE	263	5.894	21.163	50.412	1.000	13.73	
ANISOU	1787	N	PHE	263	1497	1573	2148	5	-64	1 8 6
ATOM	1788	CA	PHE	263	5.762	21.411	48.994	1.000	13.04	
ANISOU	1788	CA	PHE	263	1654	1196	2105	-12	-193	1 1 3
ATOM	1789	C	PHE	263	6.479	20.253	48.284	1.000	13.56	
ANISOU	1789	C	PHE	263	1432	1351	2370	-175	-98	-8 7
ATOM	1790	O	PHE	263	7.732	20.177	48.281	1.000	13.83	
ANISOU	1790	O	PHE	263	1415	1437	2403	-82	-299	-1 0 4
ATOM	1791	CB	PHE	263	6.364	22.770	48.594	1.000	13.50	
ANISOU	1791	CB	PHE	263	1658	1374	2098	-295	-97	3 4
ATOM	1792	CG	PHE	263	6.062	23.148	47.135	1.000	13.34	
ANISOU	1792	CG	PHE	263	1616	1358	2096	-159	-111	8 2
ATOM	1793	CD1	PHE	263	6.750	22.635	46.051	1.000	14.95	
ANISOU	1793	CD1	PHE	263	1977	1547	2156	-354	-131	-3 8 4
ATOM	1794	CD2	PHE	263	5.005	24.048	46.883	1.000	15.37	
ANISOU	1794	CD2	PHE	263	1549	1557	2735	-139	-264	3 0 3
ATOM	1795	CE1	PHE	263	6.468	22.945	44.720	1.000	14.58	
ANISOU	1795	CE1	PHE	263	1721	1621	2196	-242	71	-1 4 4
ATOM	1796	CE2	PHE	263	4.703	24.366	45.566	1.000	14.71	
ANISOU	1796	CE2	PHE	263	1482	1428	2680	-20	-261	1 3 7
ATOM	1797	CZ	PHE	263	5.383	23.809	44.479	1.000	16.55	
ANISOU	1797	CZ	PHE	263	1935	1492	2862	-152	29	1 4
ATOM	1798	N	PHE	264	5.721	19.405	47.588	1.000	12.07	
ANISOU	1798	N	PHE	264	1277	1343	1967	-66	-49	1 9
ATOM	1799	CA	PHE	264	6.267	18.328	46.769	1.000	11.90	
ANISOU	1799	CA	PHE	264	1177	1289	2058	-129	34	-2 1
ATOM	1800	C	PHE	264	6.440	18.775	45.314	1.000	11.76	

- 72 -

ANISOU	1800	C	PHE	264	1206	1258	2004	-121	-42	8
ATOM	1801	O	PHE	264	5.418	19.097	44.683	1.000	12.55	
ANISOU	1801	O	PHE	264	1165	1473	2133	-77	-120	4 6
ATOM	1802	CB	PHE	264	5.346	17.099	46.773	1.000	12.39	
ANISOU	1802	CB	PHE	264	1101	1498	2110	-304	-42	6 3
ATOM	1803	CG	PHE	264	5.022	16.558	48.150	1.000	13.97	
ANISOU	1803	CG	PHE	264	1647	1465	2197	-290	13	1 2 1
ATOM	1804	CD1	PHE	264	5.960	15.848	48.852	1.000	17.07	
ANISOU	1804	CD1	PHE	264	2039	1976	2471	-422	-410	4 9 7
ATOM	1805	CD2	PHE	264	3.747	16.679	48.668	1.000	17.41	
ANISOU	1805	CD2	PHE	264	1835	2359	2419	-440	433	1 1 2
ATOM	1806	CE1	PHE	264	5.661	15.247	50.053	1.000	20.59	
ANISOU	1806	CE1	PHE	264	2616	2710	2496	-556	-425	7 2 5
ATOM	1807	CE2	PHE	264	3.458	16.133	49.906	1.000	22.51	
ANISOU	1807	CE2	PHE	264	2151	4047	2355	-787	106	5 5 3
ATOM	1808	CZ	PHE	264	4.386	15.350	50.562	1.000	20.88	
ANISOU	1808	CZ	PHE	264	2889	2376	2669	-936	-22	3 0 6
ATOM	1809	N	LEU	265	7.676	18.756	44.811	1.000	11.81	
ANISOU	1809	N	LEU	265	1192	1248	2047	-37	47	1 9
ATOM	1810	CA	LEU	265	7.900	19.000	43.374	1.000	12.01	
ANISOU	1810	CA	LEU	265	1264	1269	2028	-223	16	- 6 3
ATOM	1811	C	LEU	265	7.915	17.617	42.703	1.000	12.10	
ANISOU	1811	C	LEU	265	1266	1298	2033	-117	-81	3
ATOM	1812	O	LEU	265	8.842	16.834	42.915	1.000	12.93	
ANISOU	1812	O	LEU	265	1367	1283	2260	-107	-152	4 4
ATOM	1813	CB	LEU	265	9.246	19.730	43.156	1.000	12.59	
ANISOU	1813	CB	LEU	265	1399	1364	2019	-257	57	- 9
ATOM	1814	CG	LEU	265	9.500	20.124	41.709	1.000	12.19	
ANISOU	1814	CG	LEU	265	1168	1399	2066	-292	-248	3 0 2
ATOM	1815	CD1	LEU	265	8.620	21.314	41.318	1.000	13.29	
ANISOU	1815	CD1	LEU	265	1518	1546	1984	84	36	1 9
ATOM	1816	CD2	LEU	265	10.971	20.458	41.449	1.000	13.14	
ANISOU	1816	CD2	LEU	265	1204	1593	2197	-234	41	- 2 0
ATOM	1817	N	ARG	266	6.842	17.249	41.996	1.000	12.06	
ANISOU	1817	N	ARG	266	1412	1127	2043	-220	-190	4 5
ATOM	1818	CA	ARG	266	6.586	15.913	41.488	1.000	12.07	
ANISOU	1818	CA	ARG	266	1372	1201	2012	-258	0	8 0
ATOM	1819	C	ARG	266	6.619	15.965	39.972	1.000	11.75	
ANISOU	1819	C	ARG	266	1203	1315	1948	29	-267	1 4 2
ATOM	1820	O	ARG	266	6.032	16.860	39.396	1.000	13.06	
ANISOU	1820	O	ARG	266	1430	1318	2214	5	-173	2 8 1
ATOM	1821	CB	ARG	266	5.243	15.370	41.994	1.000	12.95	
ANISOU	1821	CB	ARG	266	1142	1477	2302	-189	43	- 3 3
ATOM	1822	CG	ARG	266	5.036	15.606	43.488	1.000	13.80	
ANISOU	1822	CG	ARG	266	1351	1686	2207	-159	66	-11 5
ATOM	1823	CD	ARG	266	3.723	15.041	43.993	1.000	12.70	
ANISOU	1823	CD	ARG	266	1369	1362	2094	66	-22	8 4
ATOM	1824	NE	ARG	266	2.581	15.648	43.281	1.000	12.97	
ANISOU	1824	NE	ARG	266	1343	1155	2428	52	-165	-13 7
ATOM	1825	CZ	ARG	266	1.304	15.281	43.500	1.000	11.34	
ANISOU	1825	CZ	ARG	266	1432	1009	1869	45	-149	-10 3
ATOM	1826	NH1	ARG	266	0.995	14.414	44.476	1.000	13.39	
ANISOU	1826	NH1	ARG	266	1802	1165	2119	-11	-38	7 2
ATOM	1827	NH2	ARG	266	0.305	15.821	42.826	1.000	12.55	
ANISOU	1827	NH2	ARG	266	1490	1067	2210	125	-357	-15 9
ATOM	1828	N	PRO	267	7.237	14.951	39.357	1.000	12.74	
ANISOU	1828	N	PRO	267	1418	1394	2030	16	-146	1 0 8
ATOM	1829	CA	PRO	267	7.298	14.947	37.887	1.000	13.88	
ANISOU	1829	CA	PRO	267	1442	1786	2047	167	-125	- 8 4
ATOM	1830	C	PRO	267	5.957	14.722	37.222	1.000	12.61	
ANISOU	1830	C	PRO	267	1413	1508	1868	-6	44	2 7

- 73 -

ATOM	1831	O	PRO	267	4.998	14.155	37.772	1.000	13.60
ANISOU	1831	O	PRO	267	1648	1355	2164	-160	118 9 3
ATOM	1832	CB	PRO	267	8.238	13.761	37.599	1.000	15.30
ANISOU	1832	CB	PRO	267	1435	1740	2637	115	-28 -1 6 9
ATOM	1833	CG	PRO	267	8.033	12.846	38.764	1.000	15.82
ANISOU	1833	CG	PRO	267	1885	1804	2324	381	-270 -1 9 7
ATOM	1834	CD	PRO	267	7.872	13.746	39.965	1.000	14.73
ANISOU	1834	CD	PRO	267	1803	1356	2438	311	-666 -2 0 5
ATOM	1835	N	ASN	268	5.933	15.051	35.939	1.000	13.27
ANISOU	1835	N	ASN	268	1601	1665	1777	-126	-43 -1 2 7
ATOM	1836	CA	ASN	268	4.800	14.709	35.073	1.000	13.72
ANISOU	1836	CA	ASN	268	1793	1401	2018	-214	-236 -7 1
ATOM	1837	C	ASN	268	4.723	13.192	34.875	1.000	13.14
ANISOU	1837	C	ASN	268	1485	1350	2156	-213	104 5 4
ATOM	1838	O	ASN	268	5.702	12.467	34.934	1.000	13.90
ANISOU	1838	O	ASN	268	1698	1416	2167	-91	123 -3 6
ATOM	1839	CB	ASN	268	4.997	15.338	33.690	1.000	15.74
ANISOU	1839	CB	ASN	268	2597	1369	2016	-66	-437 1 3 5
ATOM	1840	CG	ASN	268	5.011	16.862	33.811	1.000	15.41
ANISOU	1840	CG	ASN	268	2255	1439	2162	-17	-184 4 7
ATOM	1841	OD1	ASN	268	4.069	17.454	34.352	1.000	17.75
ANISOU	1841	OD1	ASN	268	2573	1686	2487	42 91	-9 8
ATOM	1842	ND2	ASN	268	6.066	17.503	33.319	1.000	16.61
ANISOU	1842	ND2	ASN	268	2408	1355	2546	-50	-57 1 4 2
ATOM	1843	N	ALA	269	3.531	12.712	34.594	1.000	13.99
ANISOU	1843	N	ALA	269	1677	1467	2172	-356	-65 1 7 0
ATOM	1844	CA	ALA	269	3.278	11.286	34.353	1.000	13.42
ANISOU	1844	CA	ALA	269	1459	1405	2234	-208	-118 1 0 7
ATOM	1845	C	ALA	269	4.182	10.729	33.252	1.000	13.93
ANISOU	1845	C	ALA	269	1289	1538	2466	-168	-5 1 5 3
ATOM	1846	O	ALA	269	4.581	9.550	33.318	1.000	14.97
ANISOU	1846	O	ALA	269	1718	1476	2494	-143	112 8 6
ATOM	1847	CB	ALA	269	1.806	11.051	34.008	1.000	13.76
ANISOU	1847	CB	ALA	269	1300	1474	2454	-60	-61 1 2 3
ATOM	1848	N	ASP	270	4.482	11.541	32.251	1.000	14.38
ANISOU	1848	N	ASP	270	1688	1476	2300	-151	30 -5
ATOM	1849	CA	ASP	270	5.247	11.079	31.098	1.000	14.83
ANISOU	1849	CA	ASP	270	1747	1693	2194	-99	-42 6 8
ATOM	1850	C	ASP	270	6.749	11.287	31.227	1.000	15.68
ANISOU	1850	C	ASP	270	1714	1886	2357	-224	143 8 6
ATOM	1851	O	ASP	270	7.483	11.008	30.255	1.000	17.12
ANISOU	1851	O	ASP	270	1952	2354	2200	-80	139 2 2 6
ATOM	1852	CB	ASP	270	4.718	11.681	29.800	1.000	17.67
ANISOU	1852	CB	ASP	270	2461	1966	2288	-75	-319 1 2 6
ATOM	1853	CG	ASP	270	4.968	13.168	29.649	1.000	18.22
ANISOU	1853	CG	ASP	270	2284	2024	2613	-88	-80 4 7 4
ATOM	1854	OD1	ASP	270	5.386	13.826	30.607	1.000	20.55
ANISOU	1854	OD1	ASP	270	3424	1541	2844	-47	-287 4 2 5
ATOM	1855	OD2	ASP	270	4.646	13.698	28.552	1.000	23.06
ANISOU	1855	OD2	ASP	270	3317	2727	2719	-49	-136 8 1 2
ATOM	1856	N	PHE	271	7.221	11.668	32.413	1.000	13.93
ANISOU	1856	N	PHE	271	1556	1318	2417	97 31	4 1
ATOM	1857	CA	PHE	271	8.671	11.723	32.644	1.000	14.41
ANISOU	1857	CA	PHE	271	1624	1430	2423	110	29 2 6 3
ATOM	1858	C	PHE	271	9.275	10.349	32.325	1.000	13.31
ANISOU	1858	C	PHE	271	1402	1430	2225	-30	28 2 1 8
ATOM	1859	O	PHE	271	8.790	9.340	32.870	1.000	14.91
ANISOU	1859	O	PHE	271	1900	1374	2392	-26	240 1 9 2
ATOM	1860	CB	PHE	271	8.942	12.146	34.098	1.000	15.57
ANISOU	1860	CB	PHE	271	1700	1721	2495	-66	-36 9
ATOM	1861	CG	PHE	271	10.386	11.791	34.516	1.000	14.56

- 74 -

ANISOU	1861	CG	PHE	271	1729	1320	2485	-152	34	-124
ATOM	1862	CD1	PHE	271	11.460	12.369	33.814	1.000	17.76	
ANISOU	1862	CD1	PHE	271	1714	1581	3452	-235	393	-249
ATOM	1863	CD2	PHE	271	10.698	10.972	35.570	1.000	18.04	
ANISOU	1863	CD2	PHE	271	2182	1543	3130	-95	-540	172
ATOM	1864	CE1	PHE	271	12.786	12.092	34.166	1.000	17.54	
ANISOU	1864	CE1	PHE	271	1838	1700	3128	-291	114	-50
ATOM	1865	CE2	PHE	271	11.997	10.609	35.899	1.000	18.84	
ANISOU	1865	CE2	PHE	271	1935	1646	3578	-392	-396	425
ATOM	1866	CZ	PHE	271	13.039	11.154	35.162	1.000	17.25	
ANISOU	1866	CZ	PHE	271	2444	1697	2415	-486	-19	-394
ATOM	1867	N	THR	272	10.278	10.298	31.453	1.000	13.78	
ANISOU	1867	N	THR	272	1514	1641	2083	30	19	154
ATOM	1868	CA	THR	272	10.811	9.046	30.938	1.000	13.99	
ANISOU	1868	CA	THR	272	1551	1660	2105	-99	83	67
ATOM	1869	C	THR	272	12.246	8.841	31.410	1.000	14.71	
ANISOU	1869	C	THR	272	1598	1549	2441	-3	108	357
ATOM	1870	O	THR	272	13.046	9.808	31.424	1.000	16.23	
ANISOU	1870	O	THR	272	1646	1742	2780	-246	5	185
ATOM	1871	CB	THR	272	10.751	9.117	29.388	1.000	16.27	
ANISOU	1871	CB	THR	272	1856	2205	2119	191	125	8
ATOM	1872	OG1	THR	272	9.341	9.221	29.032	1.000	17.99	
ANISOU	1872	OG1	THR	272	1996	2473	2368	64	-190	264
ATOM	1873	CG2	THR	272	11.249	7.856	28.723	1.000	17.94	
ANISOU	1873	CG2	THR	272	2423	2167	2227	173	177	-94
ATOM	1874	N	PHE	273	12.567	7.600	31.743	1.000	14.91	
ANISOU	1874	N	PHE	273	1644	1521	2499	92	238	218
ATOM	1875	CA	PHE	273	13.894	7.253	32.254	1.000	15.16	
ANISOU	1875	CA	PHE	273	1602	1813	2345	296	277	55
ATOM	1876	C	PHE	273	14.350	5.899	31.724	1.000	14.69	
ANISOU	1876	C	PHE	273	1408	1647	2528	24	479	178
ATOM	1877	O	PHE	273	13.541	5.086	31.262	1.000	15.91	
ANISOU	1877	O	PHE	273	1738	1767	2541	-115	450	119
ATOM	1878	CB	PHE	273	13.899	7.301	33.769	1.000	15.77	
ANISOU	1878	CB	PHE	273	1758	1921	2314	-344	286	123
ATOM	1879	CG	PHE	273	12.931	6.336	34.424	1.000	14.54	
ANISOU	1879	CG	PHE	273	1390	1726	2410	-95	-11	195
ATOM	1880	CD1	PHE	273	11.601	6.743	34.655	1.000	16.64	
ANISOU	1880	CD1	PHE	273	1457	2343	2521	-24	308	362
ATOM	1881	CD2	PHE	273	13.295	5.038	34.721	1.000	15.23	
ANISOU	1881	CD2	PHE	273	1863	1624	2300	-110	91	136
ATOM	1882	CE1	PHE	273	10.719	5.848	35.259	1.000	16.10	
ANISOU	1882	CE1	PHE	273	1593	2158	2365	-162	292	122
ATOM	1883	CE2	PHE	273	12.419	4.148	35.354	1.000	16.01	
ANISOU	1883	CE2	PHE	273	1904	1980	2198	-139	285	181
ATOM	1884	CZ	PHE	273	11.109	4.559	35.548	1.000	15.18	
ANISOU	1884	CZ	PHE	273	1843	2001	1925	-141	73	-227
ATOM	1885	N	SER	274	15.634	5.612	31.926	1.000	15.31	
ANISOU	1885	N	SER	274	1559	1940	2317	361	383	247
ATOM	1886	CA	SER	274	16.221	4.318	31.518	1.000	15.37	
ANISOU	1886	CA	SER	274	1476	1723	2642	32	557	156
ATOM	1887	C	SER	274	15.953	3.284	32.588	1.000	14.67	
ANISOU	1887	C	SER	274	973	1877	2726	-113	265	302
ATOM	1888	O	SER	274	16.310	3.476	33.770	1.000	15.98	
ANISOU	1888	O	SER	274	1668	1677	2728	126	143	193
ATOM	1889	CB	SER	274	17.742	4.556	31.356	1.000	17.41	
ANISOU	1889	CB	SER	274	1487	2019	3112	235	945	725
ATOM	1890	OG	SER	274	18.362	3.280	31.334	1.000	18.03	
ANISOU	1890	OG	SER	274	1839	1961	3052	293	840	188
ATOM	1891	N	VAL	275	15.395	2.133	32.182	1.000	15.58	
ANISOU	1891	N	VAL	275	1646	1857	2417	-182	461	261

- 75 -

ATOM	1892	CA	VAL	275	15.158	1.033	33.137	1.000	15.65	
ANISOU	1892	CA	VAL	275	1681	1800	2466	-180	261	2 6 5
ATOM	1893	C	VAL	275	16.454	0.445	33.659	1.000	15.33	
ANISOU	1893	C	VAL	275	1805	1881	2139	116	392	- 4 5
ATOM	1894	O	VAL	275	16.623	0.280	34.871	1.000	15.68	
ANISOU	1894	O	VAL	275	2037	1655	2267	6	297	1 9 6
ATOM	1895	CB	VAL	275	14.227	-0.004	32.483	1.000	16.05	
ANISOU	1895	CB	VAL	275	1635	1708	2755	-76	405	2 1
ATOM	1896	CG1	VAL	275	14.080	-1.186	33.426	1.000	17.04	
ANISOU	1896	CG1	VAL	275	2045	1688	2740	-211	230	1 5
ATOM	1897	CG2	VAL	275	12.847	0.608	32.203	1.000	18.45	
ANISOU	1897	CG2	VAL	275	1650	2432	2928	-57	135	2 6 9
ATOM	1898	N	PRO	276	17.437	0.093	32.844	1.000	16.21	
ANISOU	1898	N	PRO	276	1927	1700	2532	97	589	3 6
ATOM	1899	CA	PRO	276	18.707	-0.434	33.399	1.000	18.10	
ANISOU	1899	CA	PRO	276	1736	2115	3025	147	616	- 9 3
ATOM	1900	C	PRO	276	19.382	0.541	34.321	1.000	17.52	
ANISOU	1900	C	PRO	276	1998	1961	2697	97	469	2 3 9
ATOM	1901	O	PRO	276	19.963	0.171	35.348	1.000	19.66	
ANISOU	1901	O	PRO	276	2015	2409	3047	24	280	4 6 8
ATOM	1902	CB	PRO	276	19.590	-0.796	32.214	1.000	20.80	
ANISOU	1902	CB	PRO	276	2094	2687	3121	306	771	- 2 4 9
ATOM	1903	CG	PRO	276	18.852	-0.390	30.999	1.000	21.57	
ANISOU	1903	CG	PRO	276	2051	3098	3046	340	802	- 2 8 8
ATOM	1904	CD	PRO	276	17.446	-0.021	31.368	1.000	18.17	
ANISOU	1904	CD	PRO	276	2053	2306	2546	179	832	- 3 1 8
ATOM	1905	N	LEU	277	19.325	1.845	34.027	1.000	17.09	
ANISOU	1905	N	LEU	277	1571	1898	3025	230	511	1 0 7
ATOM	1906	CA	LEU	277	19.962	2.802	34.940	1.000	19.34	
ANISOU	1906	CA	LEU	277	2035	2141	3171	-219	218	2 6 2
ATOM	1907	C	LEU	277	19.214	2.858	36.249	1.000	18.34	
ANISOU	1907	C	LEU	277	1963	1958	3049	-33	-3	- 3 8
ATOM	1908	O	LEU	277	19.815	2.957	37.319	1.000	19.29	
ANISOU	1908	O	LEU	277	2466	1710	3154	-271	-188	- 2
ATOM	1909	CB	LEU	277	20.094	4.178	34.291	1.000	21.41	
ANISOU	1909	CB	LEU	277	2739	2011	3383	14	12	2 8 7
ATOM	1910	CG	LEU	277	20.910	5.192	35.111	1.000	26.34	
ANISOU	1910	CG	LEU	277	3662	2367	3978	-980	-547	9 4 4
ATOM	1911	CD1	LEU	277	22.396	4.839	35.069	1.000	38.04	
ANISOU	1911	CD1	LEU	277	3764	3171	7518	-487	-2057	8 5 3
ATOM	1912	CD2	LEU	277	20.708	6.607	34.631	1.000	31.98	
ANISOU	1912	CD2	LEU	277	4023	2018	6109	-366	508	7 3 2
ATOM	1913	N	ALA	278	17.875	2.711	36.202	1.000	17.30	
ANISOU	1913	N	ALA	278	2015	1766	2793	74	218	1 1 5
ATOM	1914	CA	ALA	278	17.124	2.712	37.464	1.000	16.75	
ANISOU	1914	CA	ALA	278	2200	1566	2600	216	146	- 2
ATOM	1915	C	ALA	278	17.575	1.523	38.313	1.000	16.31	
ANISOU	1915	C	ALA	278	1849	1553	2794	-337	-196	1 0 7
ATOM	1916	O	ALA	278	17.718	1.635	39.523	1.000	17.26	
ANISOU	1916	O	ALA	278	1963	1839	2754	-62	-53	2 0 5
ATOM	1917	CB	ALA	278	15.642	2.622	37.177	1.000	17.55	
ANISOU	1917	CB	ALA	278	2109	1880	2679	295	195	- 1 1
ATOM	1918	N	ARG	279	17.724	0.362	37.696	1.000	17.07	
ANISOU	1918	N	ARG	279	2322	1399	2766	-178	26	3 0 8
ATOM	1919	CA	ARG	279	18.099	-0.829	38.473	1.000	16.93	
ANISOU	1919	CA	ARG	279	2377	1734	2323	15	-241	2 0 3
ATOM	1920	C	ARG	279	19.477	-0.587	39.098	1.000	19.87	
ANISOU	1920	C	ARG	279	2491	2292	2766	-487	-384	5 4 3
ATOM	1921	O	ARG	279	19.687	-0.974	40.234	1.000	33.04	
ANISOU	1921	O	ARG	279	3615	4823	4115	-1726	-1700	2 6 0 3
ATOM	1922	CB	ARG	279	18.164	-2.042	37.517	1.000	20.04	

- 76 -

ANISOU	1922	CB	ARG	279	2042	1609	3964	108	-221	-305
ATOM	1923	CG	ARG	279	16.742	-2.491	37.179	1.000	20.73	
ANISOU	1923	CG	ARG	279	2152	2728	2997	-98	-401	-351
ATOM	1924	CD	ARG	279	16.601	-3.422	35.990	1.000	24.81	
ANISOU	1924	CD	ARG	279	3213	2982	3231	-1	-507	-609
ATOM	1925	NE	ARG	279	17.575	-4.484	36.195	1.000	27.50	
ANISOU	1925	NE	ARG	279	4331	2656	3463	355	-146	-181
ATOM	1926	CZ	ARG	279	17.301	-5.725	36.620	1.000	41.33	
ANISOU	1926	CZ	ARG	279	7720	2466	5519	-186	-454	-142
ATOM	1927	NH1	ARG	279	16.024	-6.012	36.866	1.000	40.58	
ANISOU	1927	NH1	ARG	279	8821	3012	3585	-1564	507	452
ATOM	1928	NH2	ARG	279	18.200	-6.688	36.807	1.000	53.27	
ANISOU	1928	NH2	ARG	279	9516	2227	8496	-127	-4607	-463
ATOM	1929	N	GLU	280	20.390	0.119	38.424	1.000	19.68	
ANISOU	1929	N	GLU	280	2172	2276	3028	84	324	136
ATOM	1930	CA	GLU	280	21.748	0.334	38.948	1.000	20.28	
ANISOU	1930	CA	GLU	280	2046	2274	3385	25	581	115
ATOM	1931	C	GLU	280	21.705	1.257	40.182	1.000	20.67	
ANISOU	1931	C	GLU	280	2334	1968	3552	-281	285	20
ATOM	1932	O	GLU	280	22.723	1.079	40.908	1.000	26.81	
ANISOU	1932	O	GLU	280	2659	3419	4107	-37	-183	-87
ATOM	1933	CB	GLU	280	22.651	1.029	37.926	1.000	24.69	
ANISOU	1933	CB	GLU	280	2778	2558	4044	-351	1022	303
ATOM	1934	CG	GLU	280	22.997	0.342	36.634	1.000	27.13	
ANISOU	1934	CG	GLU	280	2605	4888	2816	596	116	623
ATOM	1935	CD	GLU	280	23.815	1.298	35.760	1.000	43.10	
ANISOU	1935	CD	GLU	280	4693	7780	3903	-1328	1206	834
ATOM	1936	OE1	GLU	280	24.541	2.171	36.296	1.000	41.36	
ANISOU	1936	OE1	GLU	280	2666	6033	7015	27	1099	690
ATOM	1937	OE2	GLU	280	23.727	1.219	34.520	1.000	64.81	
ANISOU	1937	OE2	GLU	280	10844	10028	3751	-2356	1104	2134
ATOM	1938	N	CYS	281	20.777	2.156	40.313	1.000	21.61	
ANISOU	1938	N	CYS	281	2372	2240	3599	-211	532	-238
ATOM	1939	CA	CYS	281	20.481	3.164	41.337	1.000	24.33	
ANISOU	1939	CA	CYS	281	2114	2911	4219	-526	1121	-817
ATOM	1940	C	CYS	281	19.858	2.568	42.585	1.000	27.11	
ANISOU	1940	C	CYS	281	2492	3261	4546	-1608	1457	-1343
ATOM	1941	O	CYS	281	19.789	3.161	43.685	1.000	19.19	
ANISOU	1941	O	CYS	281	1997	2012	3282	-250	-326	135
ATOM	1942	CB	CYS	281	19.632	4.438	40.795	1.000	22.02	
ANISOU	1942	CB	CYS	281	1214	3088	4063	-286	100	-2108
ATOM	1943	SG	CYS	281	20.639	5.092	39.444	1.000	53.41	
ANISOU	1943	SG	CYS	281	10822	4742	4730	-3261	1316	45
ATOM	1944	N	GLY	282	19.370	1.317	42.565	1.000	18.81	
ANISOU	1944	N	GLY	282	1230	2224	3695	3	-149	-206
ATOM	1945	CA	GLY	282	18.675	0.750	43.744	1.000	17.07	
ANISOU	1945	CA	GLY	282	1544	1771	3171	31	-552	-168
ATOM	1946	C	GLY	282	17.194	0.496	43.538	1.000	14.91	
ANISOU	1946	C	GLY	282	1601	1645	2417	-135	-453	378
ATOM	1947	O	GLY	282	16.480	-0.062	44.380	1.000	16.38	
ANISOU	1947	O	GLY	282	1998	1921	2306	-211	-399	360
ATOM	1948	N	PHE	283	16.625	0.919	42.404	1.000	13.44	
ANISOU	1948	N	PHE	283	1563	1539	2006	-189	-336	-115
ATOM	1949	CA	PHE	283	15.173	0.829	42.203	1.000	14.52	
ANISOU	1949	CA	PHE	283	1677	1410	2428	-187	-670	46
ATOM	1950	C	PHE	283	14.810	-0.604	41.809	1.000	13.08	
ANISOU	1950	C	PHE	283	1519	1314	2137	-121	-338	174
ATOM	1951	O	PHE	283	15.311	-1.184	40.837	1.000	14.11	
ANISOU	1951	O	PHE	283	1366	1418	2578	-142	-78	17
ATOM	1952	CB	PHE	283	14.749	1.800	41.078	1.000	13.76	
ANISOU	1952	CB	PHE	283	1814	1288	2125	-39	-268	0

- 77 -

ATOM	1953	CG	PHE	283	14.842	3.269	41.512	1.000	14.75
ANISOU	1953	CG	PHE	283	1985	1363	2255	12	-317 - 3
ATOM	1954	CD1	PHE	283	13.814	3.904	42.142	1.000	21.50
ANISOU	1954	CD1	PHE	283	2318	1759	4091	303	-23 -6 2 6
ATOM	1955	CD2	PHE	283	15.994	3.999	41.298	1.000	17.72
ANISOU	1955	CD2	PHE	283	2526	1244	2963	-307	-89 2 7 2
ATOM	1956	CE1	PHE	283	13.909	5.177	42.655	1.000	20.78
ANISOU	1956	CE1	PHE	283	2056	1802	4036	92 66	-6 4 7
ATOM	1957	CE2	PHE	283	16.115	5.290	41.814	1.000	15.06
ANISOU	1957	CE2	PHE	283	2101	1257	2364	-5	-255 3 7 7
ATOM	1958	CZ	PHE	283	15.084	5.891	42.506	1.000	18.04
ANISOU	1958	CZ	PHE	283	1881	1995	2979	192	-432 2 0
ATOM	1959	N	ASP	284	13.883	-1.178	42.579	1.000	13.07
ANISOU	1959	N	ASP	284	1549	1366	2049	-73	-331 1 1 7
ATOM	1960	CA	ASP	284	13.502	-2.584	42.395	1.000	12.80
ANISOU	1960	CA	ASP	284	1481	1460	1924	-231	-207 1 5 7
ATOM	1961	C	ASP	284	12.335	-2.654	41.421	1.000	12.88
ANISOU	1961	C	ASP	284	1493	1508	1891	-19	-180 - 5 5
ATOM	1962	O	ASP	284	11.231	-3.147	41.741	1.000	13.69
ANISOU	1962	O	ASP	284	1407	1351	2442	-93	-281 9 2
ATOM	1963	CB	ASP	284	13.141	-3.203	43.744	1.000	14.10
ANISOU	1963	CB	ASP	284	1966	1534	1858	-40	-11 1 4 5
ATOM	1964	CG	ASP	284	13.165	-4.730	43.717	1.000	14.49
ANISOU	1964	CG	ASP	284	1906	1520	2079	47	-424 2 9 0
ATOM	1965	OD1	ASP	284	13.732	-5.305	42.758	1.000	14.81
ANISOU	1965	OD1	ASP	284	2036	1343	2250	-152	-166 2 3 1
ATOM	1966	OD2	ASP	284	12.652	-5.310	44.696	1.000	15.32
ANISOU	1966	OD2	ASP	284	1979	1557	2286	-79	-109 1 5 3
ATOM	1967	N	VAL	285	12.644	-2.191	40.217	1.000	12.40
ANISOU	1967	N	VAL	285	1582	1260	1870	79	-185 - 1 3 1
ATOM	1968	CA	VAL	285	11.599	-2.064	39.216	1.000	12.31
ANISOU	1968	CA	VAL	285	1442	1469	1767	-161	-59 - 1
ATOM	1969	C	VAL	285	11.229	-3.419	38.589	1.000	12.09
ANISOU	1969	C	VAL	285	1220	1407	1967	-1	-100 - 7 9
ATOM	1970	O	VAL	285	12.085	-4.311	38.433	1.000	13.68
ANISOU	1970	O	VAL	285	1237	1514	2446	67 56 4 0	
ATOM	1971	CB	VAL	285	12.009	-1.066	38.098	1.000	14.68
ANISOU	1971	CB	VAL	285	1943	1621	2014	-163	-50 2 5 9
ATOM	1972	CG1	VAL	285	12.131	0.332	38.672	1.000	17.08
ANISOU	1972	CG1	VAL	285	2429	1402	2658	18	-465 4 2 5
ATOM	1973	CG2	VAL	285	13.309	-1.499	37.433	1.000	15.69
ANISOU	1973	CG2	VAL	285	2131	2180	1649	-316	161 3 0 6
ATOM	1974	N	SER	286	9.952	-3.541	38.241	1.000	12.24
ANISOU	1974	N	SER	286	1263	1440	1946	-12	-148 - 1 1 7
ATOM	1975	CA	SER	286	9.398	-4.669	37.495	1.000	12.84
ANISOU	1975	CA	SER	286	1571	1463	1845	-356	-30 1 4
ATOM	1976	C	SER	286	8.861	-4.118	36.172	1.000	11.99
ANISOU	1976	C	SER	286	1516	1374	1666	-28	60 - 1 9 8
ATOM	1977	O	SER	286	7.654	-4.110	35.917	1.000	15.68
ANISOU	1977	O	SER	286	1514	2384	2059	2	18 - 2 0
ATOM	1978	CB	SER	286	8.301	-5.327	38.300	1.000	12.54
ANISOU	1978	CB	SER	286	1407	1442	1915	-59	170 - 5 5
ATOM	1979	OG	SER	286	7.415	-4.380	38.890	1.000	13.15
ANISOU	1979	OG	SER	286	1531	1430	2034	105	-73 - 5 9
ATOM	1980	N	LEU	287	9.769	-3.649	35.333	1.000	13.56
ANISOU	1980	N	LEU	287	1574	1521	2058	41	133 1 7 7
ATOM	1981	CA	LEU	287	9.451	-2.932	34.101	1.000	13.48
ANISOU	1981	CA	LEU	287	1812	1418	1891	-84	116 1 7
ATOM	1982	C	LEU	287	10.075	-3.654	32.908	1.000	15.12
ANISOU	1982	C	LEU	287	1945	1714	2086	32	233 - 3 1
ATOM	1983	O	LEU	287	11.277	-3.883	32.927	1.000	17.91

- 78 -

ANISOU	1983	O	LEU	287	1885	2275	2645	109	300	-275
ATOM	1984	CB	LEU	287	9.954	-1.480	34.118	1.000	14.37	
ANISOU	1984	CB	LEU	287	1773	1380	2306	-34	248	107
ATOM	1985	CG	LEU	287	9.362	-0.603	35.231	1.000	14.32	
ANISOU	1985	CG	LEU	287	1421	1496	2523	62	52	-158
ATOM	1986	CD1	LEU	287	10.143	0.705	35.413	1.000	14.53	
ANISOU	1986	CD1	LEU	287	1672	1444	2403	0	-146	143
ATOM	1987	CD2	LEU	287	7.921	-0.197	34.820	1.000	16.03	
ANISOU	1987	CD2	LEU	287	1476	2035	2579	166	-100	-7
ATOM	1988	N	ASP	288	9.256	-4.060	31.958	1.000	15.09	
ANISOU	1988	N	ASP	288	2041	1611	2081	73	175	-216
ATOM	1989	CA	ASP	288	9.764	-4.722	30.757	1.000	16.55	
ANISOU	1989	CA	ASP	288	1992	2028	2268	29	335	-314
ATOM	1990	C	ASP	288	10.437	-3.682	29.874	1.000	18.74	
ANISOU	1990	C	ASP	288	2484	2597	2040	-231	97	81
ATOM	1991	O	ASP	288	9.998	-2.526	29.849	1.000	25.48	
ANISOU	1991	O	ASP	288	3382	2433	3865	-322	639	346
ATOM	1992	CB	ASP	288	8.659	-5.490	30.060	1.000	19.23	
ANISOU	1992	CB	ASP	288	2431	2414	2460	-209	258	-720
ATOM	1993	CG	ASP	288	9.139	-6.468	29.000	1.000	19.50	
ANISOU	1993	CG	ASP	288	2688	2223	2499	-49	393	-552
ATOM	1994	OD1	ASP	288	10.173	-7.145	29.185	1.000	27.03	
ANISOU	1994	OD1	ASP	288	3134	3038	4100	624	427	-716
ATOM	1995	OD2	ASP	288	8.458	-6.566	27.955	1.000	31.00	
ANISOU	1995	OD2	ASP	288	3596	4859	3325	307	-361	-2100
ATOM	1996	N	GLY	289	11.489	-4.035	29.137	1.000	22.68	
ANISOU	1996	N	GLY	289	2960	2893	2765	-531	778	116
ATOM	1997	CA	GLY	289	12.008	-3.083	28.169	1.000	25.60	
ANISOU	1997	CA	GLY	289	3678	3562	2486	-1469	558	11
ATOM	1998	C	GLY	289	12.988	-2.078	28.725	1.000	21.08	
ANISOU	1998	C	GLY	289	2567	2916	2528	-485	353	150
ATOM	1999	O	GLY	289	13.411	-2.097	29.891	1.000	23.72	
ANISOU	1999	O	GLY	289	3428	3219	2364	-1104	440	113
ATOM	2000	N	GLU	290	13.402	-1.168	27.818	1.000	18.32	
ANISOU	2000	N	GLU	290	2246	2396	2319	-145	616	-115
ATOM	2001	CA	GLU	290	14.538	-0.301	28.074	1.000	17.75	
ANISOU	2001	CA	GLU	290	1912	2419	2412	97	770	-367
ATOM	2002	C	GLU	290	14.261	1.058	28.696	1.000	17.90	
ANISOU	2002	C	GLU	290	2180	2308	2313	50	711	-297
ATOM	2003	O	GLU	290	15.143	1.619	29.353	1.000	17.58	
ANISOU	2003	O	GLU	290	2525	2050	2104	-35	380	165
ATOM	2004	CB	GLU	290	15.341	-0.161	26.785	1.000	23.21	
ANISOU	2004	CB	GLU	290	3184	2508	3126	-273	1753	-467
ATOM	2005	CG	GLU	290	15.833	-1.492	26.226	1.000	24.55	
ANISOU	2005	CG	GLU	290	3609	2992	2725	348	1232	-743
ATOM	2006	CD	GLU	290	16.676	-2.280	27.221	1.000	30.03	
ANISOU	2006	CD	GLU	290	3365	3708	4337	476	753	-211
ATOM	2007	OE1	GLU	290	17.492	-1.684	27.947	1.000	40.04	
ANISOU	2007	OE1	GLU	290	5043	6674	3498	525	36	-1226
ATOM	2008	OE2	GLU	290	16.622	-3.527	27.237	1.000	51.76	
ANISOU	2008	OE2	GLU	290	8785	3812	7070	-12	-483	1583
ATOM	2009	N	THR	291	13.064	1.578	28.486	1.000	18.14	
ANISOU	2009	N	THR	291	2305	2486	2103	224	711	-321
ATOM	2010	CA	THR	291	12.697	2.896	29.049	1.000	18.72	
ANISOU	2010	CA	THR	291	2521	2080	2511	105	1131	66
ATOM	2011	C	THR	291	11.278	2.744	29.593	1.000	15.79	
ANISOU	2011	C	THR	291	2178	1758	2064	134	538	-50
ATOM	2012	O	THR	291	10.517	1.834	29.217	1.000	18.62	
ANISOU	2012	O	THR	291	2764	1966	2344	-248	664	-311
ATOM	2013	CB	THR	291	12.722	4.031	28.044	1.000	21.54	
ANISOU	2013	CB	THR	291	3043	2625	2516	-164	891	362

- 79 -

ATOM	2014	OG1	THR	291	11.695	3.862	27.077	1.000	25.98	
ANISOU	2014	OG1	THR	291	3160	4072	2641	-86	703	5 0 3
ATOM	2015	CG2	THR	291	14.048	4.115	27.292	1.000	24.20	
ANISOU	2015	CG2	THR	291	3199	3832	2164	-445	930	5 3 3
ATOM	2016	N	ALA	292	10.959	3.658	30.492	1.000	14.84	
ANISOU	2016	N	ALA	292	1637	1656	2347	200	429	-1 5 3
ATOM	2017	CA	ALA	292	9.675	3.657	31.179	1.000	13.84	
ANISOU	2017	CA	ALA	292	1488	1477	2294	170	299	7 8
ATOM	2018	C	ALA	292	9.356	5.065	31.619	1.000	12.65	
ANISOU	2018	C	ALA	292	1334	1564	1908	60	144	-1 3 9
ATOM	2019	O	ALA	292	10.228	5.939	31.710	1.000	14.27	
ANISOU	2019	O	ALA	292	1529	1596	2295	-35	109	1 1 6
ATOM	2020	CB	ALA	292	9.670	2.754	32.414	1.000	14.02	
ANISOU	2020	CB	ALA	292	1693	1580	2053	37	22	-2 7
ATOM	2021	N	THR	293	8.054	5.258	31.916	1.000	13.54	
ANISOU	2021	N	THR	293	1468	1617	2058	117	373	-1 1 8
ATOM	2022	CA	THR	293	7.605	6.546	32.424	1.000	13.40	
ANISOU	2022	CA	THR	293	1565	1647	1877	152	209	-2 3 2
ATOM	2023	C	THR	293	7.407	6.482	33.952	1.000	12.09	
ANISOU	2023	C	THR	293	1345	1322	1927	-62	326	-1 2
ATOM	2024	O	THR	293	7.214	5.441	34.555	1.000	12.93	
ANISOU	2024	O	THR	293	1385	1356	2170	-190	194	9 0
ATOM	2025	CB	THR	293	6.295	7.058	31.788	1.000	13.45	
ANISOU	2025	CB	THR	293	1598	1579	1935	95	345	3 4 5
ATOM	2026	OG1	THR	293	5.273	6.112	32.117	1.000	13.75	
ANISOU	2026	OG1	THR	293	1672	1570	1981	-12	314	1 3 5
ATOM	2027	CG2	THR	293	6.476	7.139	30.272	1.000	15.93	
ANISOU	2027	CG2	THR	293	2121	2022	1911	255	434	3 3 7
ATOM	2028	N	PHE	294	7.241	7.661	34.544	1.000	12.81	
ANISOU	2028	N	PHE	294	1607	1440	1822	-83	149	-1 5 1
ATOM	2029	CA	PHE	294	6.857	7.773	35.935	1.000	12.37	
ANISOU	2029	CA	PHE	294	1332	1469	1899	-267	166	-2 8 9
ATOM	2030	C	PHE	294	5.556	7.022	36.184	1.000	12.36	
ANISOU	2030	C	PHE	294	1336	1361	1999	-151	30	-3 6
ATOM	2031	O	PHE	294	5.403	6.253	37.143	1.000	13.27	
ANISOU	2031	O	PHE	294	1556	1410	2076	-191	183	4 6
ATOM	2032	CB	PHE	294	6.698	9.271	36.267	1.000	13.83	
ANISOU	2032	CB	PHE	294	2039	1351	1866	-192	-29	-1 7 7
ATOM	2033	CG	PHE	294	6.306	9.488	37.711	1.000	13.10	
ANISOU	2033	CG	PHE	294	1786	1216	1974	-125	-63	-2 4 4
ATOM	2034	CD1	PHE	294	7.207	9.411	38.749	1.000	17.41	
ANISOU	2034	CD1	PHE	294	2132	2533	1952	-1012	-287	7 6
ATOM	2035	CD2	PHE	294	4.964	9.739	38.026	1.000	18.41	
ANISOU	2035	CD2	PHE	294	2156	2263	2575	565	332	5 7
ATOM	2036	CE1	PHE	294	6.810	9.608	40.054	1.000	17.72	
ANISOU	2036	CE1	PHE	294	2348	2296	2086	-308	-362	-1 3 6
ATOM	2037	CE2	PHE	294	4.591	10.010	39.324	1.000	19.37	
ANISOU	2037	CE2	PHE	294	2078	2541	2740	330	232	-6 3 0
ATOM	2038	CZ	PHE	294	5.507	9.956	40.355	1.000	18.36	
ANISOU	2038	CZ	PHE	294	2443	1678	2855	-394	-55	-2 4 5
ATOM	2039	N	GLN	295	4.588	7.205	35.246	1.000	12.59	
ANISOU	2039	N	GLN	295	1248	1429	2106	-62	38	-1 6 8
ATOM	2040	CA	GLN	295	3.320	6.484	35.408	1.000	12.76	
ANISOU	2040	CA	GLN	295	1266	1215	2365	7	-157	-1 1 7
ATOM	2041	C	GLN	295	3.512	4.984	35.318	1.000	12.24	
ANISOU	2041	C	GLN	295	1449	1256	1944	10	1	-7 3
ATOM	2042	O	GLN	295	2.922	4.238	36.101	1.000	13.61	
ANISOU	2042	O	GLN	295	1323	1427	2424	7	85	1 5 5
ATOM	2043	CB	GLN	295	2.375	6.975	34.317	1.000	14.31	
ANISOU	2043	CB	GLN	295	1227	1594	2616	81	-133	1 9 2
ATOM	2044	CG	GLN	295	1.062	6.256	34.249	1.000	14.03	

- 80 -

ANISOU	2044	CG	GLN	295	1391	1509	2430	-59	-300	4	7
ATOM	2045	CD	GLN	295	0.157	6.687	33.115	1.000	13.56		
ANISOU	2045	CD	GLN	295	1305	1486	2361	133	-117	1	6 5
ATOM	2046	OE1	GLN	295	0.459	7.693	32.419	1.000	15.35		
ANISOU	2046	OE1	GLN	295	1811	1651	2371	161	206	2	2 0
ATOM	2047	NE2	GLN	295	-0.982	6.026	32.943	1.000	15.04		
ANISOU	2047	NE2	GLN	295	1225	1995	2493	75	-139	-	9 9
ATOM	2048	N	ASP	296	4.363	4.463	34.423	1.000	12.66		
ANISOU	2048	N	ASP	296	1425	1396	1990	181	-112	-	1 1 0
ATOM	2049	CA	ASP	296	4.653	3.016	34.439	1.000	12.26		
ANISOU	2049	CA	ASP	296	1628	1274	1755	53	-51	-	1 5 1
ATOM	2050	C	ASP	296	5.167	2.569	35.792	1.000	11.57		
ANISOU	2050	C	ASP	296	1199	1300	1895	-82	30	-	2 2
ATOM	2051	O	ASP	296	4.854	1.460	36.224	1.000	13.08		
ANISOU	2051	O	ASP	296	1534	1368	2070	-107	38	1	3 9
ATOM	2052	CB	ASP	296	5.709	2.634	33.399	1.000	14.18		
ANISOU	2052	CB	ASP	296	1870	1700	1819	141	30	-	3 7 8
ATOM	2053	CG	ASP	296	5.295	2.848	31.952	1.000	13.32		
ANISOU	2053	CG	ASP	296	1655	1557	1848	-58	67	2	
ATOM	2054	OD1	ASP	296	4.110	2.725	31.601	1.000	15.83		
ANISOU	2054	OD1	ASP	296	1680	1935	2402	-68	-126	-	1 8 9
ATOM	2055	OD2	ASP	296	6.212	3.098	31.114	1.000	15.27		
ANISOU	2055	OD2	ASP	296	1757	1937	2106	-229	137	1	7 7
ATOM	2056	N	TRP	297	6.038	3.352	36.416	1.000	12.26		
ANISOU	2056	N	TRP	297	1325	1403	1931	-34	-123	-	1 1 8
ATOM	2057	CA	TRP	297	6.683	2.960	37.656	1.000	12.82		
ANISOU	2057	CA	TRP	297	1328	1599	1943	-104	-49	1	5 1
ATOM	2058	C	TRP	297	5.746	3.007	38.858	1.000	13.13		
ANISOU	2058	C	TRP	297	1418	1580	1992	24	-23	1	8 5
ATOM	2059	O	TRP	297	5.565	2.030	39.584	1.000	14.03		
ANISOU	2059	O	TRP	297	1554	1619	2159	102	137	3	2 0
ATOM	2060	CB	TRP	297	7.908	3.847	37.928	1.000	13.68		
ANISOU	2060	CB	TRP	297	1130	1692	2376	-19	-169	1	5 1
ATOM	2061	CG	TRP	297	8.646	3.455	39.166	1.000	13.28		
ANISOU	2061	CG	TRP	297	1143	1646	2255	91	-96	2	2
ATOM	2062	CD1	TRP	297	8.932	2.179	39.622	1.000	15.58		
ANISOU	2062	CD1	TRP	297	1615	1689	2618	275	-544	-	7 7
ATOM	2063	CD2	TRP	297	9.144	4.353	40.189	1.000	14.69		
ANISOU	2063	CD2	TRP	297	1327	1693	2562	-117	-219	5	
ATOM	2064	NE1	TRP	297	9.583	2.265	40.840	1.000	15.34		
ANISOU	2064	NE1	TRP	297	1378	1853	2598	70	-494	7	5
ATOM	2065	CE2	TRP	297	9.724	3.597	41.203	1.000	16.13		
ANISOU	2065	CE2	TRP	297	1241	2009	2880	182	-676	-	1 9 6
ATOM	2066	CE3	TRP	297	9.094	5.756	40.284	1.000	22.13		
ANISOU	2066	CE3	TRP	297	3040	1658	3712	-665	-1408	1	2 9
ATOM	2067	CZ2	TRP	297	10.318	4.180	42.316	1.000	18.45		
ANISOU	2067	CZ2	TRP	297	2204	2387	2418	44	-326	-	3 3 1
ATOM	2068	CZ3	TRP	297	9.670	6.353	41.399	1.000	21.55		
ANISOU	2068	CZ3	TRP	297	2916	2104	3167	-55	-752	-	4 5 8
ATOM	2069	CH2	TRP	297	10.258	5.546	42.397	1.000	23.53		
ANISOU	2069	CH2	TRP	297	3298	2356	3285	-320	-1146	-	3 4 4
ATOM	2070	N	ILE	298	5.106	4.167	39.044	1.000	13.58		
ANISOU	2070	N	ILE	298	1324	1726	2108	241	-167	1	2 7
ATOM	2071	CA	ILE	298	4.299	4.440	40.229	1.000	14.68		
ANISOU	2071	CA	ILE	298	1413	2177	1986	-13	-161	-	2 0 8
ATOM	2072	C	ILE	298	2.841	4.054	40.121	1.000	12.02		
ANISOU	2072	C	ILE	298	1455	1300	1813	56	-239	4	0 2
ATOM	2073	O	ILE	298	2.182	3.782	41.147	1.000	13.67		
ANISOU	2073	O	ILE	298	1732	1582	1881	-23	-4	1	9 3
ATOM	2074	CB	ILE	298	4.428	5.914	40.673	1.000	19.45		
ANISOU	2074	CB	ILE	298	2261	2446	2683	-699	237	-	8 3 5

- 81 -

ATOM	2075	CG1	ILE	298	5.907	6.245	41.001	1.000	27.83
ANISOU	2075	CG1	ILE	298	2776	4275	3525	-1314	-556 -1030
ATOM	2076	CG2	ILE	298	3.679	6.319	41.929	1.000	25.05
ANISOU	2076	CG2	ILE	298	3770	3344	2405	-57	255 -983
ATOM	2077	CD1	ILE	298	6.368	5.628	42.306	1.000	43.32
ANISOU	2077	CD1	ILE	298	4561	7224	4674	-652	-1890 -117
ATOM	2078	N	GLY	299	2.317	3.980	38.893	1.000	12.16
ANISOU	2078	N	GLY	299	1432	1308	1879	78 -304	106
ATOM	2079	CA	GLY	299	0.918	3.741	38.670	1.000	12.98
ANISOU	2079	CA	GLY	299	1276	1279	2379	106	-188 -154
ATOM	2080	C	GLY	299	0.135	5.017	38.378	1.000	13.09
ANISOU	2080	C	GLY	299	1421	1403	2151	113	-231 118
ATOM	2081	O	GLY	299	0.738	6.025	38.017	1.000	14.00
ANISOU	2081	O	GLY	299	1713	1353	2252	122	289 -13
ATOM	2082	N	GLY	300	-1.183	4.917	38.447	1.000	13.08
ANISOU	2082	N	GLY	300	1325	1545	2099	146	-267 -145
ATOM	2083	CA	GLY	300	-2.075	5.966	37.992	1.000	13.45
ANISOU	2083	CA	GLY	300	1447	1521	2143	116	-415 -143
ATOM	2084	C	GLY	300	-2.519	6.972	39.042	1.000	12.94
ANISOU	2084	C	GLY	300	1098	1365	2456	-52	-407 -192
ATOM	2085	O	GLY	300	-3.262	7.875	38.672	1.000	13.39
ANISOU	2085	O	GLY	300	1321	1342	2423	-19	-217 -45
ATOM	2086	N	ASN	301	-1.973	6.845	40.254	1.000	13.35
ANISOU	2086	N	ASN	301	1494	1429	2151	-225	-232 -104
ATOM	2087	CA	ASN	301	-2.162	7.842	41.313	1.000	13.83
ANISOU	2087	CA	ASN	301	1590	1435	2230	-194	-38 -61
ATOM	2088	C	ASN	301	-0.837	8.254	41.885	1.000	12.46
ANISOU	2088	C	ASN	301	1676	1268	1791	-35	-142 -20
ATOM	2089	O	ASN	301	-0.007	7.405	42.169	1.000	13.89
ANISOU	2089	O	ASN	301	1831	1355	2093	73 -144	-13
ATOM	2090	CB	ASN	301	-3.075	7.238	42.360	1.000	16.01
ANISOU	2090	CB	ASN	301	1632	1909	2542	77 224	315
ATOM	2091	CG	ASN	301	-3.942	8.199	43.106	1.000	18.23
ANISOU	2091	CG	ASN	301	1986	2508	2435	190	152 -90
ATOM	2092	OD1	ASN	301	-4.973	8.690	42.614	1.000	17.44
ANISOU	2092	OD1	ASN	301	1606	1626	3394	-21	144 -190
ATOM	2093	ND2	ASN	301	-3.518	8.454	44.338	1.000	33.30
ANISOU	2093	ND2	ASN	301	2804	6923	2928	1012	-230 -1523
ATOM	2094	N	TYR	302	-0.595	9.564	42.073	1.000	12.96
ANISOU	2094	N	TYR	302	1662	1278	1985	-69	-21 -135
ATOM	2095	CA	TYR	302	0.674	9.948	42.702	1.000	13.48
ANISOU	2095	CA	TYR	302	1673	1259	2192	-130	-132 34
ATOM	2096	C	TYR	302	0.768	9.269	44.078	1.000	12.63
ANISOU	2096	C	TYR	302	1413	1293	2092	53 44	19
ATOM	2097	O	TYR	302	-0.218	9.151	44.806	1.000	14.15
ANISOU	2097	O	TYR	302	1332	1737	2305	-65	48 -27
ATOM	2098	CB	TYR	302	0.764	11.472	42.916	1.000	13.30
ANISOU	2098	CB	TYR	302	1635	1192	2226	-81	33 41
ATOM	2099	CG	TYR	302	1.159	12.143	41.619	1.000	12.02
ANISOU	2099	CG	TYR	302	1586	1103	1880	-59	-25 -271
ATOM	2100	CD1	TYR	302	2.501	12.233	41.275	1.000	13.11
ANISOU	2100	CD1	TYR	302	1633	1284	2066	-80	11 -18
ATOM	2101	CD2	TYR	302	0.235	12.709	40.739	1.000	12.52
ANISOU	2101	CD2	TYR	302	1576	1132	2049	-44	13 -127
ATOM	2102	CE1	TYR	302	2.933	12.822	40.119	1.000	12.29
ANISOU	2102	CE1	TYR	302	1581	1043	2045	-185	-84 -77
ATOM	2103	CE2	TYR	302	0.637	13.273	39.535	1.000	14.12
ANISOU	2103	CE2	TYR	302	1462	1443	2458	-241	15 325
ATOM	2104	CZ	TYR	302	1.983	13.347	39.241	1.000	12.69
ANISOU	2104	CZ	TYR	302	1483	1224	2113	-287	-91 10
ATOM	2105	OH	TYR	302	2.376	13.866	38.013	1.000	13.42

- 82 -

ANISOU	2105	OH	TYR	302	1505	1469	2124	-93	33	1	4	6
ATOM	2106	N	VAL	303	1.956	8.855	44.450	1.000	13	9	2	
ANISOU	2106	N	VAL	303	1406	1637	2246	153	88	9	9	
ATOM	2107	CA	VAL	303	2.355	8.336	45.746	1.000	14	5	1	
ANISOU	2107	CA	VAL	303	1838	1320	2355	-137	-391	-7	4	
ATOM	2108	C	VAL	303	3.498	9.244	46.239	1.000	15	2	3	
ANISOU	2108	C	VAL	303	1404	1507	2876	-102	-105	-3	4	8
ATOM	2109	O	VAL	303	4.471	9.386	45.512	1.000	18	7	0	
ANISOU	2109	O	VAL	303	1859	1861	3386	-239	326	-5	0	4
ATOM	2110	CB	VAL	303	2.856	6.880	45.632	1.000	16	7	5	
ANISOU	2110	CB	VAL	303	2140	1319	2905	16	-759	-1	2	3
ATOM	2111	CG1	VAL	303	3.279	6.401	47.017	1.000	19	5	3	
ANISOU	2111	CG1	VAL	303	2185	1951	3284	232	-1054	1	4	8
ATOM	2112	CG2	VAL	303	1.723	5.956	45.125	1.000	17	8	2	
ANISOU	2112	CG2	VAL	303	2476	1442	2852	-213	-558	-4	0	6
ATOM	2113	N	ASN	304	3.349	9.900	47.378	1.000	14	0	7	
ANISOU	2113	N	ASN	304	1409	1369	2566	-39	-407	-8	6	
ATOM	2114	CA	ASN	304	4.317	10.928	47.772	1.000	14	3	1	
ANISOU	2114	CA	ASN	304	1474	1387	2578	-102	-424	-5	5	
ATOM	2115	C	ASN	304	5.450	10.397	48.637	1.000	13	7	5	
ANISOU	2115	C	ASN	304	1360	1487	2378	34	-274	-8	7	
ATOM	2116	O	ASN	304	6.539	10.962	48.584	1.000	14	6	0	
ANISOU	2116	O	ASN	304	1314	1795	2438	-34	-55	-3	2	0
ATOM	2117	CB	ASN	304	3.589	12.035	48.551	1.000	14	2	6	
ANISOU	2117	CB	ASN	304	1710	1214	2494	6	-303	1	7	6
ATOM	2118	CG	ASN	304	2.535	12.661	47.642	1.000	14	8	1	
ANISOU	2118	CG	ASN	304	1551	1627	2449	23	-114	4	0	2
ATOM	2119	OD1	ASN	304	2.866	13.255	46.622	1.000	16	5	2	
ANISOU	2119	OD1	ASN	304	1896	1746	2636	80	19	5	8	9
ATOM	2120	ND2	ASN	304	1.290	12.595	48.102	1.000	18	4	3	
ANISOU	2120	ND2	ASN	304	1560	2980	2463	127	-10	1	9	9
ATOM	2121	N	ILE	305	5.175	9.413	49.463	1.000	16	3	6	
ANISOU	2121	N	ILE	305	1546	1553	3117	-78	-503	2	6	6
ATOM	2122	CA	ILE	305	6.173	8.890	50.407	1.000	14	8	5	
ANISOU	2122	CA	ILE	305	1670	1537	2436	165	-277	-4	0	
ATOM	2123	C	ILE	305	6.183	7.372	50.352	1.000	15	7	8	
ANISOU	2123	C	ILE	305	1527	1555	2914	95	-438	-5	1	
ATOM	2124	O	ILE	305	5.231	6.736	49.886	1.000	17	5	4	
ANISOU	2124	O	ILE	305	1463	1789	3412	-131	-404	5		
ATOM	2125	CB	ILE	305	5.949	9.430	51.818	1.000	17	8	0	
ANISOU	2125	CB	ILE	305	2167	1962	2634	-23	265	-2	0	9
ATOM	2126	CG1	ILE	305	4.578	9.091	52.416	1.000	18	9	3	
ANISOU	2126	CG1	ILE	305	1716	2948	2526	1	-218	-1	6	3
ATOM	2127	CG2	ILE	305	6.171	10.944	51.823	1.000	19	1	7	
ANISOU	2127	CG2	ILE	305	2685	1863	2737	70	-534	-4	0	5
ATOM	2128	CD1	ILE	305	4.415	9.459	53.863	1.000	21	2	8	
ANISOU	2128	CD1	ILE	305	2521	2902	2662	19	452	-7	1	
ATOM	2129	N	ARG	306	7.246	6.806	50.908	1.000	14	5	9	
ANISOU	2129	N	ARG	306	1738	1641	2165	52	-356	2	7	1
ATOM	2130	CA	ARG	306	7.424	5.360	50.828	1.000	15	2	5	
ANISOU	2130	CA	ARG	306	1509	1663	2622	139	-302	7	7	
ATOM	2131	C	ARG	306	8.234	4.903	52.024	1.000	15	0	2	
ANISOU	2131	C	ARG	306	1588	1464	2656	133	-332	-2	1	
ATOM	2132	O	ARG	306	9.141	5.614	52.433	1.000	16	6	3	
ANISOU	2132	O	ARG	306	1682	2101	2536	-219	-294	-1	6	8
ATOM	2133	CB	ARG	306	8.135	4.943	49.532	1.000	16	3	1	
ANISOU	2133	CB	ARG	306	1820	1681	2697	-100	-270	-1	5	0
ATOM	2134	CG	ARG	306	8.226	3.414	49.377	1.000	18	4	3	
ANISOU	2134	CG	ARG	306	2476	1700	2828	40	-194	-1	5	6
ATOM	2135	CD	ARG	306	8.401	3.068	47.900	1.000	18	2	6	
ANISOU	2135	CD	ARG	306	2087	1971	2880	-120	-145	-3	3	0

- 83 -

ATOM 2136 NE ARG 306 7.136 3.228 47.188 1.000 20.53
 ANISOU 2136 NE ARG 306 2442 2013 3345 -577 -668 -234
 ATOM 2137 CZ ARG 306 6.980 3.178 45.873 1.000 20.27
 ANISOU 2137 CZ ARG 306 2330 2057 3316 373 -522 20
 ATOM 2138 NH1 ARG 306 8.086 3.000 45.107 1.000 22.13
 ANISOU 2138 NH1 ARG 306 2136 2580 3695 274 -589 -723
 ATOM 2139 NH2 ARG 306 5.759 3.250 45.341 1.000 18.44
 ANISOU 2139 NH2 ARG 306 2107 1838 3062 259 -286 84
 ATOM 2140 N ARG 307 7.898 3.775 52.612 1.000 19.10
 ANISOU 2140 N ARG 307 2716 1872 2671 -294 -607 327
 ATOM 2141 CA ARG 307 8.576 3.212 53.768 1.000 21.13
 ANISOU 2141 CA ARG 307 3321 2201 2504 -48 -845 139
 ATOM 2142 C ARG 307 9.536 2.138 53.277 1.000 23.30
 ANISOU 2142 C ARG 307 3417 2170 3267 181 -1046 39
 ATOM 2143 O ARG 307 9.385 1.601 52.187 1.000 21.01
 ANISOU 2143 O ARG 307 2574 2355 3052 174 -728 112
 ATOM 2144 CB ARG 307 7.557 2.522 54.694 1.000 27.30
 ANISOU 2144 CB ARG 307 4545 3184 2645 -13 -247 705
 ATOM 2145 CG ARG 307 6.839 3.488 55.629 1.000 46.30
 ANISOU 2145 CG ARG 307 6310 6374 4907 215 1655 -970
 ATOM 2146 CD ARG 307 7.054 3.085 57.085 1.000 66.50
 ANISOU 2146 CD ARG 307 11107 10355 3806 -2980 2792 -1145
 ATOM 2147 NE ARG 307 5.989 2.203 57.531 1.000 78.91
 ANISOU 2147 NE ARG 307 11821 12833 5330 -4530 1969 -5
 ATOM 2148 CZ ARG 307 5.987 1.285 58.479 1.000 73.67
 ANISOU 2148 CZ ARG 307 7704 14382 5907 -4724 1249 1051
 ATOM 2149 NH1 ARG 307 7.063 1.038 59.214 1.000 80.32
 ANISOU 2149 NH1 ARG 307 6613 17949 5955 -3290 2179 105
 ATOM 2150 NH2 ARG 307 4.872 0.597 58.707 1.000 73.74
 ANISOU 2150 NH2 ARG 307 9116 15919 2983 -6954 438 -917
 ATOM 2151 N THR 308 10.551 1.861 54.113 1.000 25.61
 ANISOU 2151 N THR 308 4234 2212 3285 536 -1421 -232
 ATOM 2152 CA THR 308 11.308 0.640 53.822 1.000 30.02
 ANISOU 2152 CA THR 308 3468 1939 5998 225 -1629 -194
 ATOM 2153 C THR 308 10.468 -0.611 54.030 1.000 25.42
 ANISOU 2153 C THR 308 2915 2190 4552 453 -626 -321
 ATOM 2154 O THR 308 9.523 -0.768 54.787 1.000 30.10
 ANISOU 2154 O THR 308 4042 3482 3912 614 -217 -125
 ATOM 2155 CB THR 308 12.581 0.531 54.688 1.000 26.09
 ANISOU 2155 CB THR 308 2701 3586 3626 242 -361 -456
 ATOM 2156 OG1 THR 308 12.140 0.751 56.028 1.000 32.90
 ANISOU 2156 OG1 THR 308 4146 4188 4167 504 745 -495
 ATOM 2157 CG2 THR 308 13.577 1.594 54.256 1.000 31.43
 ANISOU 2157 CG2 THR 308 3193 4702 4047 -577 -132 -538
 ATOM 2158 N SER 309 10.850 -1.591 53.217 1.000 24.73
 ANISOU 2158 N SER 309 2934 2092 4370 94 -574 -391
 ATOM 2159 CA SER 309 10.199 -2.897 53.230 1.000 25.19
 ANISOU 2159 CA SER 309 3793 2464 3316 -485 451 -230
 ATOM 2160 C SER 309 10.466 -3.691 54.512 1.000 24.06
 ANISOU 2160 C SER 309 2360 2888 3893 302 107 35
 ATOM 2161 O SER 309 11.565 -3.621 55.084 1.000 34.54
 ANISOU 2161 O SER 309 3626 2131 7366 -76 -1944 -34
 ATOM 2162 CB SER 309 10.639 -3.700 52.012 1.000 26.52
 ANISOU 2162 CB SER 309 3970 2159 3948 167 580 -366
 ATOM 2163 OG SER 309 10.217 -5.039 52.148 1.000 26.34
 ANISOU 2163 OG SER 309 3198 2207 4604 156 -844 -260
 ATOM 2164 N LYS 310 9.494 -4.458 54.961 1.000 24.99
 ANISOU 2164 N LYS 310 3172 2459 3864 160 262 366
 ATOM 2165 CA LYS 310 9.651 -5.339 56.125 1.000 28.38
 ANISOU 2165 CA LYS 310 4191 3167 3427 764 278 281
 ATOM 2166 C LYS 310 9.941 -6.768 55.711 1.000 26.07

- 84 -

ANISOU	2166	C	LYS	310	3371	2687	3846	168	-290	5	7	7
ATOM	2167	O	LYS	310	10.150	-7.684	56.515	1.000	33	4	8	
ANISOU	2167	O	LYS	310	5267	3056	4400	-66	-450	1	0	7
ATOM	2168	CB	LYS	310	8.299	-5.367	56.858	1.000	37	7	7	
ANISOU	2168	CB	LYS	310	5736	4695	3921	299	1818	1	8	
ATOM	2169	CG	LYS	310	8.014	-4.214	57.806	1.000	40	5	5	
ANISOU	2169	CG	LYS	310	6395	4716	4295	1525	1524	1	0	1
ATOM	2170	CD	LYS	310	6.798	-4.587	58.649	1.000	44	2	4	
ANISOU	2170	CD	LYS	310	9091	4224	3495	1053	2816	5	8	4
ATOM	2171	CE	LYS	310	6.722	-6.109	58.818	1.000	59	1	2	
ANISOU	2171	CE	LYS	310	9281	4577	8606	766	-82	2	4	7
ATOM	2172	NZ	LYS	310	6.088	-6.563	60.089	1.000	55	8	0	
ANISOU	2172	NZ	LYS	310	4884	5742	10577	287	-947	4	7	9
ATOM	2173	N	ALA	311	9.896	-7.030	54.410	1.000	22	4	5	
ANISOU	2173	N	ALA	311	2190	2402	3939	10	52	2	6	9
ATOM	2174	CA	ALA	311	10.360	-8.369	53.972	1.000	31	1	8	9
ANISOU	2174	CA	ALA	311	3771	2594	5753	434	-516	-4	2	1
ATOM	2175	C	ALA	311	11.909	-8.459	53.833	1.000	23	3	0	
ANISOU	2175	C	ALA	311	3907	2328	2616	1393	-593	1	1	2
ATOM	2176	CB	ALA	311	9.619	-8.665	52.674	1.000	27	9	4	
ANISOU	2176	CB	ALA	311	2407	2878	5329	-355	542	-6	7	2
ATOM	2177	OW	HOH	501	-6.477	10.237	44.256	1.000	15	6	6	
ATOM	2178	OW	HOH	502	-9.349	16.189	51.010	1.000	19	2	6	
ATOM	2179	OW	HOH	503	-1.489	3.653	34.560	1.000	15	7	8	
ATOM	2180	OW	HOH	504	-10.499	18.731	50.182	1.000	16	1	9	
ATOM	2181	OW	HOH	505	-8.612	16.958	47.640	1.000	17	3	0	
ATOM	2182	OW	HOH	506	-10.255	20.839	42.881	1.000	19	0	5	
ATOM	2183	OW	HOH	507	2.096	1.076	32.810	1.000	29	3	2	
ATOM	2184	OW	HOH	508	-0.284	4.743	41.885	1.000	13	9	3	
ATOM	2185	OW	HOH	509	-8.525	18.553	42.416	1.000	21	3	3	
ATOM	2186	OW	HOH	510	3.165	2.604	43.488	1.000	24	5	9	
ATOM	2187	OW	HOH	511	-6.282	19.386	52.341	1.000	18	9	8	
ATOM	2188	OW	HOH	512	-6.826	24.638	46.833	1.000	21	7	7	
ATOM	2189	OW	HOH	513	10.510	-4.344	46.092	1.000	25	8	8	
ATOM	2190	OW	HOH	514	-0.806	16.964	40.372	1.000	16	5	4	
ATOM	2191	OW	HOH	515	-1.269	18.855	42.411	1.000	15	7	6	
ATOM	2192	OW	HOH	516	14.277	-5.146	40.175	1.000	15	5	3	
ATOM	2193	OW	HOH	517	-0.123	21.538	40.640	1.000	17	2	2	
ATOM	2194	OW	HOH	518	13.131	-0.967	51.791	1.000	31	1	7	
ATOM	2195	OW	HOH	519	11.009	2.875	45.599	1.000	20	2	0	
ATOM	2196	OW	HOH	520	5.789	13.543	45.996	1.000	17	3	6	
ATOM	2197	OW	HOH	521	2.168	19.767	55.925	1.000	20	4	1	
ATOM	2198	OW	HOH	522	8.487	15.960	34.949	1.000	15	4	0	
ATOM	2199	OW	HOH	523	10.794	12.697	29.921	1.000	19	9	9	
ATOM	2200	OW	HOH	524	-11.722	19.112	44.516	1.000	19	8	2	
ATOM	2201	OW	HOH	525	1.672	-2.081	35.124	1.000	16	2	9	
ATOM	2202	OW	HOH	526	9.651	15.283	32.342	1.000	20	3	7	
ATOM	2203	OW	HOH	527	28.749	31.187	52.019	1.000	18	5	3	
ATOM	2204	OW	HOH	528	15.326	11.252	32.041	1.000	19	6	0	
ATOM	2205	OW	HOH	529	26.897	26.984	52.035	1.000	19	8	6	
ATOM	2206	OW	HOH	530	13.528	11.592	50.915	1.000	16	1	7	
ATOM	2207	OW	HOH	531	25.631	32.409	52.682	1.000	19	2	0	
ATOM	2208	OW	HOH	532	18.287	6.835	52.185	1.000	18	4	9	
ATOM	2209	OW	HOH	533	12.635	29.035	39.395	1.000	18	0	9	
ATOM	2210	OW	HOH	534	10.797	31.968	45.659	1.000	20	6	6	
ATOM	2211	OW	HOH	535	10.167	24.890	33.567	1.000	19	1	2	
ATOM	2212	OW	HOH	536	23.530	24.122	58.531	1.000	20	3	9	
ATOM	2213	OW	HOH	537	23.358	12.639	35.292	1.000	22	6	1	
ATOM	2214	OW	HOH	538	25.879	28.699	50.264	1.000	19	4	4	
ATOM	2215	OW	HOH	539	11.674	16.559	30.502	1.000	18	5	7	
ATOM	2216	OW	HOH	540	18.515	27.775	40.042	1.000	22	2	3	

- 85 -

ATOM	2217	OW	HOH	541	21.233	20.367	33.996	1.000	21.45
ATOM	2218	OW	HOH	542	22.826	32.643	53.094	1.000	19.38
ATOM	2219	OW	HOH	543	19.670	22.387	35.310	1.000	20.05
ATOM	2220	OW	HOH	544	-13.591	21.996	61.494	1.000	49.93
ATOM	2221	OW	HOH	545	21.295	11.783	55.080	1.000	20.04
ATOM	2222	OW	HOH	546	5.431	2.533	51.677	1.000	28.11
ATOM	2223	OW	HOH	547	17.311	25.489	32.148	1.000	24.38
ATOM	2224	OW	HOH	548	17.427	7.744	33.008	1.000	20.78
ATOM	2225	OW	HOH	549	11.656	23.874	58.194	1.000	23.39
ATOM	2226	OW	HOH	550	8.037	14.987	53.326	1.000	33.52
ATOM	2227	OW	HOH	551	1.354	14.574	33.889	1.000	21.05
ATOM	2228	OW	HOH	552	11.203	20.116	63.686	1.000	24.59
ATOM	2229	OW	HOH	553	2.671	21.240	34.245	1.000	34.51
ATOM	2230	OW	HOH	554	6.339	19.832	30.751	1.000	26.36
ATOM	2231	OW	HOH	555	26.611	24.519	55.570	1.000	21.22
ATOM	2232	OW	HOH	556	27.669	17.156	53.039	1.000	25.86
ATOM	2233	OW	HOH	557	-14.392	19.977	44.154	1.000	25.03
ATOM	2234	OW	HOH	558	14.828	32.652	51.443	1.000	25.23
ATOM	2235	OW	HOH	559	17.937	7.207	54.915	1.000	20.59
ATOM	2236	OW	HOH	560	10.729	-8.875	31.499	1.000	24.65
ATOM	2237	OW	HOH	561	6.455	2.298	42.613	1.000	22.74
ATOM	2238	OW	HOH	562	13.784	31.245	44.166	1.000	27.75
ATOM	2239	OW	HOH	563	17.292	33.470	53.556	1.000	25.28
ATOM	2240	OW	HOH	564	11.210	1.109	49.697	1.000	23.33
ATOM	2241	OW	HOH	565	-11.339	25.246	41.370	1.000	26.08
ATOM	2242	OW	HOH	566	20.363	-8.375	38.242	1.000	30.07
ATOM	2243	OW	HOH	567	3.890	24.604	35.837	1.000	25.86
ATOM	2244	OW	HOH	568	5.334	11.875	43.937	1.000	25.45
ATOM	2245	OW	HOH	569	7.861	22.385	64.046	1.000	28.98
ATOM	2246	OW	HOH	570	7.754	-1.508	30.848	1.000	24.72
ATOM	2247	OW	HOH	571	6.297	3.583	28.471	1.000	33.06
ATOM	2248	OW	HOH	572	-15.790	28.800	51.855	1.000	30.09
ATOM	2249	OW	HOH	573	-5.388	20.310	38.883	1.000	23.64
ATOM	2250	OW	HOH	574	17.657	21.059	29.053	1.000	24.31
ATOM	2251	OW	HOH	575	8.763	20.920	66.102	1.000	24.81
ATOM	2252	OW	HOH	576	10.135	27.617	58.357	1.000	25.12
ATOM	2253	OW	HOH	577	7.795	1.060	29.730	1.000	29.00
ATOM	2254	OW	HOH	578	22.601	19.580	61.946	1.000	28.66
ATOM	2255	OW	HOH	579	8.859	4.744	27.898	1.000	26.12
ATOM	2256	OW	HOH	580	4.937	3.932	48.882	1.000	26.29
ATOM	2257	OW	HOH	581	17.096	5.891	35.057	1.000	23.31
ATOM	2258	OW	HOH	582	-16.337	31.047	64.719	1.000	54.01
ATOM	2259	OW	HOH	583	7.652	24.826	52.106	1.000	27.23
ATOM	2260	OW	HOH	584	7.174	24.915	29.292	1.000	26.60
ATOM	2261	OW	HOH	585	23.452	10.614	55.439	1.000	26.42
ATOM	2262	OW	HOH	586	12.640	26.413	58.676	1.000	27.15
ATOM	2263	OW	HOH	587	6.204	21.166	62.094	1.000	24.65
ATOM	2264	OW	HOH	588	2.385	0.810	37.616	1.000	19.92
ATOM	2265	OW	HOH	589	32.930	28.236	45.738	1.000	38.29
ATOM	2266	OW	HOH	590	-12.045	28.716	45.065	1.000	30.46
ATOM	2267	OW	HOH	591	0.219	13.612	36.120	1.000	27.12
ATOM	2268	OW	HOH	592	-2.525	3.881	43.344	1.000	26.67
ATOM	2269	OW	HOH	593	7.533	13.297	48.055	1.000	19.59
ATOM	2270	OW	HOH	594	-1.575	28.355	42.057	1.000	25.53
ATOM	2271	OW	HOH	595	11.209	-1.188	46.425	1.000	22.12
ATOM	2272	OW	HOH	596	5.684	-7.000	28.451	1.000	27.97
ATOM	2273	OW	HOH	597	28.868	19.406	51.825	1.000	27.72
ATOM	2274	OW	HOH	598	13.432	2.493	57.904	1.000	31.12
ATOM	2275	OW	HOH	599	8.196	7.483	27.148	1.000	29.99
ATOM	2276	OW	HOH	600	20.809	19.088	63.369	1.000	36.86
ATOM	2277	OW	HOH	601	21.352	10.656	34.614	1.000	30.60

- 86 -

ATOM	2278	OW	HOH	602	2.891	7.196	30.899	1.000	25.41
ATOM	2279	OW	HOH	603	8.260	26.496	34.561	1.000	35.71
ATOM	2280	OW	HOH	604	22.300	13.959	31.378	1.000	32.53
ATOM	2281	OW	HOH	605	15.689	35.750	48.870	1.000	31.17
ATOM	2282	OW	HOH	606	7.219	15.638	30.914	1.000	27.80
ATOM	2283	OW	HOH	607	-3.237	14.604	47.092	1.000	20.96
ATOM	2284	OW	HOH	608	17.543	10.581	33.561	1.000	23.51
ATOM	2285	OW	HOH	609	-1.899	36.370	44.261	1.000	32.64
ATOM	2286	OW	HOH	610	26.095	14.431	43.803	1.000	19.19
ATOM	2287	OW	HOH	611	27.664	13.183	41.954	1.000	26.48
ATOM	2288	OW	HOH	612	4.302	34.604	49.981	1.000	24.70
ATOM	2289	OW	HOH	613	-15.580	27.012	46.728	1.000	42.45
ATOM	2290	OW	HOH	614	1.615	35.544	50.347	1.000	23.78
ATOM	2291	OW	HOH	615	-10.137	34.259	49.033	1.000	23.94
ATOM	2292	OW	HOH	616	26.084	6.502	57.657	1.000	39.32
ATOM	2293	OW	HOH	617	-15.962	20.656	46.340	1.000	25.94
ATOM	2294	OW	HOH	618	6.113	29.517	40.143	1.000	29.43
ATOM	2295	OW	HOH	619	19.797	4.627	51.313	1.000	27.15
ATOM	2296	OW	HOH	620	-1.748	11.315	48.716	1.000	21.83
ATOM	2297	OW	HOH	621	11.099	34.289	44.259	1.000	27.15
ATOM	2298	OW	HOH	622	28.352	14.351	37.877	1.000	41.48
ATOM	2299	OW	HOH	623	-2.826	36.968	57.149	1.000	32.75
ATOM	2300	OW	HOH	624	16.983	9.258	29.962	1.000	32.82
ATOM	2301	OW	HOH	625	16.780	29.213	38.384	1.000	27.96
ATOM	2302	OW	HOH	626	1.632	17.213	33.689	1.000	23.17
ATOM	2303	OW	HOH	627	33.536	23.640	45.028	1.000	41.91
ATOM	2304	OW	HOH	628	23.821	6.059	50.174	1.000	34.22
ATOM	2305	OW	HOH	629	3.482	2.785	46.751	1.000	39.07
ATOM	2306	OW	HOH	630	20.218	24.803	60.918	1.000	50.12
ATOM	2307	OW	HOH	631	3.366	16.272	30.698	1.000	31.50
ATOM	2308	OW	HOH	632	18.871	11.791	31.384	1.000	30.78
ATOM	2309	OW	HOH	633	4.455	25.782	58.823	1.000	32.14
ATOM	2310	OW	HOH	634	24.721	5.202	40.319	1.000	40.13
ATOM	2311	OW	HOH	635	19.623	35.238	43.466	1.000	50.48
ATOM	2312	OW	HOH	636	22.789	26.242	60.797	1.000	26.58
ATOM	2313	OW	HOH	637	7.008	-4.809	54.039	1.000	33.89
ATOM	2314	OW	HOH	638	-15.821	18.362	42.559	1.000	29.61
ATOM	2315	OW	HOH	639	-11.847	15.711	52.841	1.000	25.21
ATOM	2316	OW	HOH	640	-1.948	13.411	35.401	1.000	30.41
ATOM	2317	OW	HOH	641	-14.293	21.937	42.145	1.000	27.58
ATOM	2318	OW	HOH	642	18.216	20.839	66.863	1.000	31.23
ATOM	2319	OW	HOH	643	9.836	36.288	48.178	1.000	44.21
ATOM	2320	OW	HOH	644	3.510	16.168	66.253	1.000	33.82
ATOM	2321	OW	HOH	645	7.571	33.398	41.687	1.000	37.96
ATOM	2322	OW	HOH	646	0.780	21.844	36.729	1.000	31.71
ATOM	2323	OW	HOH	647	21.244	-2.321	35.579	1.000	32.40
ATOM	2324	OW	HOH	648	3.027	25.244	69.907	1.000	36.84
ATOM	2325	OW	HOH	649	1.129	25.273	66.516	1.000	35.42
ATOM	2326	OW	HOH	650	14.646	7.560	60.327	1.000	46.42
ATOM	2327	OW	HOH	651	-8.287	26.381	37.998	1.000	29.17
ATOM	2328	OW	HOH	652	10.153	23.548	67.703	1.000	31.50
ATOM	2329	OW	HOH	653	28.906	22.258	38.969	1.000	32.66
ATOM	2330	OW	HOH	654	13.568	-4.482	31.517	1.000	26.94
ATOM	2331	OW	HOH	655	-12.635	17.106	55.637	1.000	26.85
ATOM	2332	OW	HOH	656	2.698	5.770	50.702	1.000	29.05
ATOM	2333	OW	HOH	657	-1.384	7.487	46.512	1.000	36.52
ATOM	2334	OW	HOH	658	3.880	19.246	31.498	1.000	31.50
ATOM	2335	OW	HOH	659	-1.400	31.406	64.001	1.000	56.62
ATOM	2336	OW	HOH	660	11.416	23.260	65.229	1.000	32.69
ATOM	2337	OW	HOH	661	15.994	14.673	25.680	1.000	36.46
ATOM	2338	OW	HOH	662	28.572	21.242	53.423	1.000	39.06

- 87 -

ATOM	2339	OW	HOH	663	19.354	0.465	27.273	1.000	44.56
ATOM	2340	OW	HOH	664	24.969	27.026	38.838	1.000	35.41
ATOM	2341	OW	HOH	665	24.294	7.488	55.914	1.000	32.97
ATOM	2342	OW	HOH	666	19.540	7.882	31.178	1.000	30.04
ATOM	2343	OW	HOH	667	-9.236	32.988	57.241	1.000	39.20
ATOM	2344	OW	HOH	668	2.098	18.351	67.496	1.000	38.88
ATOM	2345	OW	HOH	669	11.390	3.245	56.270	1.000	37.56
ATOM	2346	OW	HOH	670	-21.413	24.449	52.026	1.000	44.66
ATOM	2347	OW	HOH	671	-14.575	19.220	55.240	1.000	30.91
ATOM	2348	OW	HOH	672	32.112	25.958	43.051	1.000	33.34
ATOM	2349	OW	HOH	673	-15.050	31.151	53.232	1.000	34.71
ATOM	2350	OW	HOH	674	2.941	-1.607	30.245	1.000	34.63
ATOM	2351	OW	HOH	675	26.951	14.544	34.757	1.000	49.17
ATOM	2352	OW	HOH	676	14.707	30.669	39.386	1.000	30.55
ATOM	2353	OW	HOH	677	5.203	18.009	68.080	1.000	43.41
ATOM	2354	OW	HOH	678	14.151	7.965	26.591	1.000	38.80
ATOM	2355	OW	HOH	679	24.470	24.261	41.443	1.000	31.28
ATOM	2356	OW	HOH	680	17.540	2.410	28.478	1.000	34.31
ATOM	2357	OW	HOH	681	25.992	20.593	34.326	1.000	39.66
ATOM	2358	OW	HOH	682	13.802	35.357	44.421	1.000	34.06
ATOM	2359	OW	HOH	683	1.087	2.355	45.456	1.000	35.39
ATOM	2360	OW	HOH	684	22.443	34.538	42.053	1.000	33.55
ATOM	2361	OW	HOH	685	4.419	4.720	27.356	1.000	48.02
ATOM	2362	OW	HOH	686	-15.830	34.507	51.877	1.000	50.63
ATOM	2363	OW	HOH	687	-15.217	29.490	48.887	1.000	33.54
ATOM	2364	OW	HOH	688	36.808	21.183	46.206	1.000	44.97
ATOM	2365	OW	HOH	689	3.756	1.312	29.272	1.000	35.16
ATOM	2366	OW	HOH	690	18.802	13.646	27.901	1.000	30.08
ATOM	2367	OW	HOH	691	6.997	17.521	29.313	1.000	47.70
ATOM	2368	OW	HOH	692	13.725	16.327	69.105	1.000	36.97
ATOM	2369	OW	HOH	693	22.369	22.161	60.503	1.000	44.09
ATOM	2370	OW	HOH	694	-5.429	31.620	42.219	1.000	33.40
ATOM	2371	OW	HOH	695	19.351	23.082	30.744	1.000	34.21
ATOM	2372	OW	HOH	696	6.897	22.414	29.376	1.000	36.59
ATOM	2373	OW	HOH	697	28.700	7.809	57.304	1.000	38.35
ATOM	2374	OW	HOH	698	3.224	0.679	39.819	1.000	24.13
ATOM	2375	OW	HOH	699	-4.634	33.717	62.593	1.000	32.26
ATOM	2376	OW	HOH	700	32.423	17.018	43.200	1.000	43.20
ATOM	2377	OW	HOH	701	12.119	25.228	68.342	1.000	39.95
ATOM	2378	OW	HOH	702	9.307	16.477	28.976	1.000	31.75
ATOM	2379	OW	HOH	703	-11.313	34.067	46.117	1.000	49.40
ATOM	2380	OW	HOH	704	7.774	31.390	65.371	1.000	39.12
ATOM	2381	OW	HOH	705	24.764	7.530	36.802	1.000	38.55
ATOM	2382	OW	HOH	706	-22.095	25.669	59.047	1.000	36.71
ATOM	2383	OW	HOH	707	14.509	9.840	68.854	1.000	50.38
ATOM	2384	OW	HOH	708	-10.129	28.722	42.036	1.000	38.92
ATOM	2385	OW	HOH	709	29.011	34.910	48.390	1.000	35.29
ATOM	2386	OW	HOH	710	15.822	31.612	42.021	1.000	33.61
ATOM	2387	OW	HOH	711	-1.996	17.676	33.645	1.000	49.57
ATOM	2388	OW	HOH	712	10.216	17.748	26.015	1.000	41.04
ATOM	2389	OW	HOH	713	23.535	29.642	37.371	1.000	43.47
ATOM	2390	OW	HOH	714	20.488	-7.214	35.599	1.000	45.99
ATOM	2391	OW	HOH	715	11.411	10.149	25.081	1.000	41.63
ATOM	2392	OW	HOH	716	19.329	-4.258	34.139	1.000	42.50
ATOM	2393	OW	HOH	717	13.688	26.799	66.321	1.000	43.74
ATOM	2394	OW	HOH	718	-10.751	33.064	54.747	1.000	40.47
ATOM	2395	OW	HOH	719	13.800	18.258	70.756	1.000	34.54
ATOM	2396	OW	HOH	720	17.151	5.815	28.003	1.000	40.80
ATOM	2397	OW	HOH	721	0.000	0.000	36.691	0.330	27.42
ATOM	2398	OW	HOH	722	0.000	0.000	41.559	0.330	37.77
ATOM	2399	OW	HOH	723	15.314	7.549	28.791	1.000	36.24

- 88 -

ATOM	2400	OW	HOH	724	-1.663	19.944	39.196	1.000	33.87
ATOM	2401	OW	HOH	725	19.289	24.195	33.321	1.000	32.28
ATOM	2402	OW	HOH	726	0.000	0.000	31.798	0.330	50.38
ATOM	2403	OW	HOH	727	-1.223	38.165	59.229	1.000	31.24
ATOM	2404	OW	HOH	728	22.035	38.254	45.742	1.000	48.21
ATOM	2405	OW	HOH	729	28.388	16.248	63.044	1.000	31.59
ATOM	2406	OW	HOH	730	0.000	0.000	45.995	0.330	36.14
ATOM	2407	OW	HOH	731	2.984	29.007	40.091	1.000	36.08
ATOM	2408	OW	HOH	732	5.297	15.835	27.318	1.000	41.53
ATOM	2409	OW	HOH	733	17.347	10.778	27.373	1.000	35.27
ATOM	2410	OW	HOH	734	29.417	14.607	53.127	1.000	40.12
ATOM	2411	OW	HOH	735	4.222	-8.636	27.012	1.000	35.22
ATOM	2412	OW	HOH	736	-9.949	17.712	62.813	1.000	34.43
ATOM	2413	OW	HOH	737	13.960	-10.203	55.259	1.000	31.79
ATOM	2414	OW	HOH	738	11.831	-1.522	49.308	1.000	25.22
ATOM	2415	OW	HOH	739	2.896	4.247	29.596	1.000	38.64
ATOM	2416	OW	HOH	740	10.959	13.759	25.528	1.000	61.86
ATOM	2417	OW	HOH	741	0.864	17.227	30.557	1.000	50.71
ATOM	2418	OW	HOH	742	31.755	18.949	52.065	1.000	40.48
ATOM	2419	OW	HOH	743	21.678	-0.485	28.218	1.000	43.23
ATOM	2420	OW	HOH	744	10.583	16.397	75.211	1.000	45.04
ATOM	2421	OW	HOH	745	7.480	7.996	78.287	1.000	57.64
ATOM	2422	OW	HOH	746	24.067	35.122	40.297	1.000	41.95
ATOM	2423	OW	HOH	747	7.804	10.269	78.332	1.000	49.63
ATOM	2424	OW	HOH	748	22.131	40.645	45.806	1.000	49.69
ATOM	2425	OW	HOH	749	14.850	-4.647	33.872	1.000	42.88
ATOM	2426	OW	HOH	750	-12.930	32.504	55.211	1.000	37.15
ATOM	2427	OW	HOH	751	-4.832	35.986	43.333	1.000	44.39
ATOM	2428	OW	HOH	752	19.834	33.566	56.449	1.000	31.56
ATOM	2429	OW	HOH	753	3.363	22.310	29.844	1.000	42.02
ATOM	2430	OW	HOH	754	25.594	4.030	34.174	1.000	51.90
ATOM	2431	OW	HOH	755	28.036	35.859	46.448	1.000	39.50
ATOM	2432	OW	HOH	756	-12.951	16.294	61.787	1.000	40.94
ATOM	2433	OW	HOH	757	-10.870	26.452	38.737	1.000	44.85
ATOM	2434	OW	HOH	758	13.216	12.896	70.729	1.000	63.42
ATOM	2435	OW	HOH	759	-0.403	21.161	74.990	1.000	38.96
ATOM	2436	OW	HOH	760	-7.025	32.526	64.316	1.000	39.64
ATOM	2437	OW	HOH	761	-15.459	19.739	58.090	1.000	40.84
ATOM	2438	OW	HOH	762	-4.964	36.577	59.068	1.000	48.64
ATOM	2439	OW	HOH	763	26.807	35.717	50.036	1.000	43.54
ATOM	2440	OW	HOH	764	19.542	7.083	65.538	1.000	41.41
ATOM	2441	OW	HOH	765	3.709	35.837	42.709	1.000	33.78
ATOM	2442	OW	HOH	766	0.431	33.688	40.172	1.000	36.91
ATOM	2443	OW	HOH	767	18.620	5.064	64.617	1.000	45.76
ATOM	2444	OW	HOH	768	35.526	19.792	41.322	1.000	52.54
ATOM	2445	OW	HOH	769	19.671	7.789	67.717	1.000	43.44
ATOM	2446	OW	HOH	770	3.562	12.048	26.149	1.000	40.08
ATOM	2447	OW	HOH	771	20.245	35.637	53.927	1.000	52.16
ATOM	2448	OW	HOH	772	-20.588	25.640	61.573	1.000	58.60
ATOM	2449	OW	HOH	773	1.556	37.342	52.171	1.000	36.23
ATOM	2450	OW	HOH	774	8.340	0.668	49.382	1.000	107.24
ATOM	2451	OW	HOH	775	27.160	2.372	34.466	1.000	59.84
ATOM	2452	OW	HOH	776	6.575	19.271	25.545	1.000	36.68

- 89 -

ATOM	2453	OW	HOH	777	-17.605	29.205	62.661	1.000	56.83
ATOM	2454	OW	HOH	778	7.616	6.902	24.722	1.000	61.34
ATOM	2455	OW	HOH	779	19.749	10.700	68.006	1.000	65.22
ATOM	2456	W	HOH	780	7.281	-5.270	50.090	1.000	50.00
ATOM	2457	W	HOH	781	-6.809	28.483	40.515	1.000	50.00
ATOM	2458	W	HOH	782	9.990	17.263	38.636	1.000	50.00
ATOM	2459	W	HOH	783	5.767	-2.331	28.939	1.000	50.00
ATOM	2460	W	HOH	784	11.694	-0.118	24.984	1.000	50.00
ATOM	2461	W	HOH	785	24.442	7.952	47.994	1.000	50.00
ATOM	2462	W	HOH	786	14.251	36.889	46.491	1.000	50.00
ATOM	2463	W	HOH	787	5.759	26.477	33.851	1.000	50.00
ATOM	2464	W	HOH	788	-11.816	22.606	40.795	1.000	50.00
ATOM	2465	W	HOH	789	-2.531	5.579	45.829	1.000	50.00
ATOM	2466	W	HOH	790	-13.002	32.034	46.612	1.000	50.00
ATOM	2467	W	HOH	791	2.230	3.555	48.985	1.000	50.00
ATOM	2468	W	HOH	792	9.397	13.464	28.121	1.000	50.00
ATOM	2469	W	HOH	793	28.257	10.442	42.781	1.000	50.00
ATOM	2470	W	HOH	794	4.652	17.944	59.241	1.000	50.00
ATOM	2471	W	HOH	795	5.977	15.287	79.554	1.000	50.00
ATOM	2472	W	HOH	796	30.501	11.852	47.616	1.000	50.00
ATOM	2473	W	HOH	797	5.625	14.258	54.367	1.000	50.00
ATOM	2474	W	HOH	798	23.942	20.228	33.277	1.000	50.00
ATOM	2475	W	HOH	799	10.164	14.642	58.997	1.000	50.00
ATOM	2476	W	HOH	800	7.807	31.943	52.999	1.000	50.00
ATOM	2477	W	HOH	801	23.377	9.361	34.817	1.000	50.00
ATOM	2478	W	HOH	802	21.193	9.722	32.004	1.000	50.00
ATOM	2479	W	HOH	803	34.928	14.644	46.038	1.000	50.00
ATOM	2480	W	HOH	804	29.073	16.684	34.445	1.000	50.00
ATOM	2481	W	HOH	805	7.008	-2.049	51.872	1.000	50.00
ATOM	2482	W	HOH	806	25.363	7.860	45.531	1.000	50.00
ATOM	2483	W	HOH	807	30.704	8.207	55.971	1.000	50.00
ATOM	2484	W	HOH	808	33.072	24.900	40.599	1.000	50.00
ATOM	2485	W	HOH	809	-15.577	19.225	63.152	1.000	50.00
ATOM	2486	W	HOH	810	6.072	18.137	23.603	1.000	50.00
ATOM	2487	W	HOH	811	-7.214	39.940	55.639	1.000	50.00
ATOM	2488	W	HOH	812	5.509	18.517	74.919	1.000	50.00
ATOM	2489	W	HOH	813	33.845	9.908	56.672	1.000	50.00
ATOM	2490	W	HOH	814	0.421	35.779	42.931	1.000	50.00
ATOM	2491	W	HOH	815	35.282	21.705	48.656	1.000	50.00
ATOM	2492	W	HOH	816	39.344	22.173	46.871	1.000	50.00
ATOM	2493	W	HOH	817	-5.192	39.820	60.056	1.000	50.00
ATOM	2494	W	HOH	818	30.199	13.039	33.383	1.000	50.00
ATOM	2495	W	HOH	819	-4.860	36.454	61.731	1.000	50.00
ATOM	2496	W	HOH	820	-14.599	17.407	58.382	1.000	50.00
ATOM	2497	W	HOH	821	1.340	-0.111	41.711	0.500	50.00
ATOM	2498	W	HOH	822	34.512	23.218	52.108	1.000	50.00
ATOM	2499	W	HOH	823	32.136	12.571	52.190	1.000	50.00
ATOM	2500	W	HOH	824	13.525	-6.549	29.838	1.000	50.00
ATOM	2501	W	HOH	825	6.072	-4.141	27.534	1.000	50.00

STRUCTURE B

ATOM	1	CB	MET	1	31.030	11.882	57.066	1.000	50.96		
ANISOU	1	CB	MET	1	5663	3892	9809	1113	-2217	-554	
ATOM	2	CG	MET	1	30.206	12.690	56.086	1.000	51.63		
ANISOU	2	CG	MET	1	6595	3775	9246	691	-1891	169	
ATOM	3	SD	MET	1	28.694	11.848	55.559	1.000	40.50		
ANISOU	3	SD	MET	1	7003	3962	4424	833	-1535	-460	
ATOM	4	CE	MET	1	27.852	11.584	57.120	1.000	45.32		
ANISOU	4	CE	MET	1	8632	3912	4677	-239	-653	-1702	
ATOM	5	C	MET	1	31.587	13.367	58.999	1.000	52.14		
ANISOU	5	C	MET	1	6204	4752	8854	287	-2128	-63	
ATOM	6	O	MET	1	31.239	12.847	60.058	1.000	52.92		
ANISOU	6	O	MET	1	7381	5242	7483	1417	-4224	519	
ATOM	7	N	MET	1	33.170	11.646	58.275	1.000	57.78		
ANISOU	7	N	MET	1	4533	6034	11388	34	-1912	-811	
ATOM	8	CA	MET	1	32.156	12.587	57.819	1.000	54.62		
ANISOU	8	CA	MET	1	6441	4752	9560	137	-2012	-617	
ATOM	9	N	ASP	2	31.485	14.679	58.792	1.000	43.52		
ANISOU	9	N	ASP	2	3460	4866	8210	474	-2350	47	
ATOM	10	CA	ASP	2	30.759	15.471	59.796	1.000	41.69		
ANISOU	10	CA	ASP	2	4439	4678	6722	-309	-2603	-31	
ATOM	11	CB	ASP	2	31.206	16.912	59.644	1.000	37.89		
ANISOU	11	CB	ASP	2	3805	4768	5822	-304	-3473	266	
ATOM	12	CG	ASP	2	30.219	17.958	60.121	1.000	39.59		
ANISOU	12	CG	ASP	2	4511	4616	5916	15	-3218	589	
ATOM	13	OD1	ASP	2	29.325	17.637	60.933	1.000	45.10		
ANISOU	13	OD1	ASP	2	5866	4689	6581	-553	-1950	-625	
ATOM	14	OD2	ASP	2	30.363	19.121	59.663	1.000	42.05		
ANISOU	14	OD2	ASP	2	5994	4341	5643	-465	-3788	145	
ATOM	15	C	ASP	2	29.275	15.213	59.556	1.000	33.84		
ANISOU	15	C	ASP	2	4131	3634	5094	-59	-1682	-122	
ATOM	16	O	ASP	2	28.901	15.176	58.379	1.000	29.25		
ANISOU	16	O	ASP	2	2232	4393	4489	658	-390	-615	
ATOM	17	N	THR	3	28.467	15.029	60.597	1.000	29.41		
ANISOU	17	N	THR	3	4731	2636	3807	907	-2076	-284	
ATOM	18	CA	THR	3	27.046	14.764	60.421	1.000	28.55		
ANISOU	18	CA	THR	3	4602	2494	3753	597	-1006	-390	
ATOM	19	CB	THR	3	26.447	13.762	61.414	1.000	36.51		
ANISOU	19	CB	THR	3	7170	2209	4495	-791	-1996	52	
ATOM	20	OG1	THR	3	26.629	14.220	62.758	1.000	42.45		
ANISOU	20	OG1	THR	3	9519	2620	3989	-920	-1251	383	
ATOM	21	CG2	THR	3	27.153	12.412	61.315	1.000	50.26		
ANISOU	21	CG2	THR	3	9604	1863	7630	-602	-733	-333	
ATOM	22	C	THR	3	26.240	16.061	60.553	1.000	29.01		
ANISOU	22	C	THR	3	4535	2548	3939	738	-1079	99	
ATOM	23	O	THR	3	25.041	16.044	60.827	1.000	35.82		
ANISOU	23	O	THR	3	5149	2485	5976	390	524	-1246	
ATOM	24	N	THR	4	26.928	17.181	60.332	1.000	24.98		
ANISOU	24	N	THR	4	3874	2456	3162	542	-2040	-986	
ATOM	25	CA	THR	4	26.214	18.465	60.327	1.000	23.97		
ANISOU	25	CA	THR	4	3437	2426	3244	344	-1563	-375	
ATOM	26	CB	THR	4	27.183	19.650	60.408	1.000	26.77		
ANISOU	26	CB	THR	4	2636	2429	5105	651	-988	-923	
ATOM	27	OG1	THR	4	28.050	19.484	61.551	1.000	32.62		
ANISOU	27	OG1	THR	4	3398	2812	6184	195	-2081	-1134	
ATOM	28	CG2	THR	4	26.429	20.942	60.663	1.000	26.40		
ANISOU	28	CG2	THR	4	2373	2692	4967	533	-573	-1570	
ATOM	29	C	THR	4	25.325	18.577	59.097	1.000	21.64		
ANISOU	29	C	THR	4	3090	2760	2374	368	-750	-20	
ATOM	30	O	THR	4	25.738	18.264	57.980	1.000	21.58		
ANISOU	30	O	THR	4	2668	2629	2902	246	-560	-659	
ATOM	31	N	VAL	5	24.104	19.049	59.340	1.000	15.88		

- 91 -

ANISOU 31	N	VAL	5	2505	2021	1508	-613	-630	-162
ATOM 32	CA	VAL	5	23.211	19.385	58.211	1.000	14.80	
ANISOU 32	CA	VAL	5	2463	1893	1266	-594	-473	-87
ATOM 33	CB	VAL	5	21.742	19.402	58.606	1.000	16.09	
ANISOU 33	CB	VAL	5	2476	1881	1757	-412	-406	502
ATOM 34	CG1	VAL	5	20.855	19.846	57.447	1.000	14.91	
ANISOU 34	CG1	VAL	5	2468	1859	1337	9	-102	197
ATOM 35	CG2	VAL	5	21.310	17.994	59.074	1.000	21.15	
ANISOU 35	CG2	VAL	5	3015	2345	2677	-700	-418	1198
ATOM 36	C	VAL	5	23.639	20.762	57.694	1.000	17.70	
ANISOU 36	C	VAL	5	2893	2085	1749	-1137	-713	103
ATOM 37	O	VAL	5	23.532	21.759	58.419	1.000	17.35	
ANISOU 37	O	VAL	5	2566	1978	2050	-698	-650	105
ATOM 38	N	PRO	6	24.150	20.845	56.479	1.000	13.23	
ANISOU 38	N	PRO	6	1334	1597	2097	-162	-668	409
ATOM 39	CD	PRO	6	24.302	19.770	55.484	1.000	15.56	
ANISOU 39	CD	PRO	6	1887	1850	2176	-309	-383	277
ATOM 40	CA	PRO	6	24.667	22.137	56.005	1.000	14.49	
ANISOU 40	CA	PRO	6	1332	1740	2432	-218	-536	522
ATOM 41	CB	PRO	6	25.571	21.722	54.847	1.000	18.21	
ANISOU 41	CB	PRO	6	2294	1740	2886	-224	130	434
ATOM 42	CG	PRO	6	25.132	20.378	54.409	1.000	20.37	
ANISOU 42	CG	PRO	6	2708	2632	2399	-1078	38	-61
ATOM 43	C	PRO	6	23.576	23.091	55.510	1.000	14.59	
ANISOU 43	C	PRO	6	1388	1712	2443	-406	-786	698
ATOM 44	O	PRO	6	22.408	22.743	55.295	1.000	13.06	
ANISOU 44	O	PRO	6	1298	1547	2118	-283	-596	15
ATOM 45	N	THR	7	24.048	24.326	55.313	1.000	14.56	
ANISOU 45	N	THR	7	1393	1678	2463	-380	-565	587
ATOM 46	CA	THR	7	23.288	25.428	54.771	1.000	13.28	
ANISOU 46	CA	THR	7	1463	1584	1998	-469	-734	440
ATOM 47	CB	THR	7	23.121	26.572	55.799	1.000	14.44	
ANISOU 47	CB	THR	7	1927	1652	1905	-348	-1257	329
ATOM 48	OG1	THR	7	22.454	26.102	56.998	1.000	18.44	
ANISOU 48	OG1	THR	7	3136	2013	1858	-333	-829	176
ATOM 49	CG2	THR	7	22.290	27.719	55.261	1.000	14.98	
ANISOU 49	CG2	THR	7	1390	1788	2513	-213	-727	412
ATOM 50	C	THR	7	23.973	26.005	53.539	1.000	14.62	
ANISOU 50	C	THR	7	1144	2200	2212	-355	-693	704
ATOM 51	O	THR	7	25.192	26.257	53.600	1.000	17.21	
ANISOU 51	O	THR	7	1284	2515	2738	-641	-840	975
ATOM 52	N	PHE	8	23.211	26.222	52.472	1.000	12.32	
ANISOU 52	N	PHE	8	1165	1596	1919	-314	-534	370
ATOM 53	CA	PHE	8	23.692	26.869	51.283	1.000	13.31	
ANISOU 53	CA	PHE	8	1554	1531	1971	-60	-295	343
ATOM 54	CB	PHE	8	23.724	25.933	50.067	1.000	13.71	
ANISOU 54	CB	PHE	8	1479	1705	2025	-136	-232	234
ATOM 55	CG	PHE	8	24.635	24.746	50.258	1.000	13.68	
ANISOU 55	CG	PHE	8	1225	1716	2257	-185	8	155
ATOM 56	CD1	PHE	8	24.147	23.503	50.628	1.000	14.10	
ANISOU 56	CD1	PHE	8	1317	1710	2329	-93	231	221
ATOM 57	CD2	PHE	8	26.006	24.882	50.079	1.000	17.52	
ANISOU 57	CD2	PHE	8	1239	2282	3134	-234	-56	917
ATOM 58	CE1	PHE	8	24.984	22.420	50.812	1.000	15.39	
ANISOU 58	CE1	PHE	8	1473	1878	2497	-11	242	481
ATOM 59	CE2	PHE	8	26.840	23.807	50.271	1.000	17.73	
ANISOU 59	CE2	PHE	8	1179	2259	3301	-157	-143	423
ATOM 60	CZ	PHE	8	26.348	22.567	50.654	1.000	17.12	
ANISOU 60	CZ	PHE	8	1310	2437	2757	24	-382	978
ATOM 61	C	PHE	8	22.821	28.073	50.909	1.000	12.76	
ANISOU 61	C	PHE	8	1401	1513	1935	-164	-145	442

- 92 -

ATOM	62	O	PHE	8	21.602	28.033	51.079	1.000	13.18
ANISOU	62	O	PHE	8	1392	1295	2322	-256	-400 3 6 4
ATOM	63	N	SER	9	23.478	29.096	50.394	1.000	13.03
ANISOU	63	N	SER	9	1722	1636	1593	-565	-601 4 9 0
ATOM	64	CA	SER	9	22.861	30.224	49.718	1.000	12.55
ANISOU	64	CA	SER	9	1591	1468	1708	-392	-438 3 1 5
ATOM	65	CB	SER	9	23.743	31.472	49.761	1.000	15.41
ANISOU	65	CB	SER	9	2385	1833	1637	-915	-1057 7 8 3
ATOM	66	OG	SER	9	23.138	32.539	49.007	1.000	17.99
ANISOU	66	OG	SER	9	2504	1721	2611	-718	-999 9 2 4
ATOM	67	C	SER	9	22.520	29.868	48.276	1.000	12.72
ANISOU	67	C	SER	9	2040	1187	1606	-411	-576 4 7 6
ATOM	68	O	SER	9	23.397	29.495	47.478	1.000	16.18
ANISOU	68	O	SER	9	2265	2053	1830	-465	-381 7 3
ATOM	69	N	LEU	10	21.229	29.982	47.968	1.000	14.19
ANISOU	69	N	LEU	10	2154	1488	1750	-301	-699 1 7 4
ATOM	70	CA	LEU	10	20.798	29.714	46.596	1.000	14.62
ANISOU	70	CA	LEU	10	2243	1579	1734	-184	-784 2 2 4
ATOM	71	CB	LEU	10	19.291	29.883	46.436	1.000	14.72
ANISOU	71	CB	LEU	10	2222	1714	1657	-142	-657 -1 6 8
ATOM	72	CG	LEU	10	18.693	29.633	45.050	1.000	14.10
ANISOU	72	CG	LEU	10	2087	1557	1713	-702	-695 1 4 5
ATOM	73	CD1	LEU	10	18.986	28.214	44.582	1.000	16.23
ANISOU	73	CD1	LEU	10	2994	1578	1595	-554	-1132 8 7
ATOM	74	CD2	LEU	10	17.198	29.913	44.997	1.000	21.82
ANISOU	74	CD2	LEU	10	2180	2904	3206	-421	-1151 -5 1 8
ATOM	75	C	LEU	10	21.531	30.639	45.626	1.000	15.87
ANISOU	75	C	LEU	10	2449	1785	1796	-491	-844 3 1 4
ATOM	76	O	LEU	10	21.962	30.199	44.553	1.000	16.33
ANISOU	76	O	LEU	10	2607	1816	1780	-601	-829 2 7 6
ATOM	77	N	ALA	11	21.669	31.917	45.986	1.000	17.17
ANISOU	77	N	ALA	11	2521	1889	2115	-607	-548 1 3 9
ATOM	78	CA	ALA	11	22.335	32.912	45.129	1.000	16.56
ANISOU	78	CA	ALA	11	2377	1884	2029	-732	-1033 3 0 2
ATOM	79	CB	ALA	11	22.199	34.259	45.805	1.000	20.05
ANISOU	79	CB	ALA	11	3210	1877	2529	-670	-674 2 5 9
ATOM	80	C	ALA	11	23.786	32.535	44.831	1.000	16.33
ANISOU	80	C	ALA	11	2319	2255	1629	-754	-988 4 3 4
ATOM	81	O	ALA	11	24.260	32.587	43.677	1.000	19.66
ANISOU	81	O	ALA	11	3115	2559	1795	-947	-560 6 1 9
ATOM	82	N	GLU	12	24.558	32.085	45.810	1.000	17.28
ANISOU	82	N	GLU	12	2686	1994	1884	-454	-1087 3 9 0
ATOM	83	CA	GLU	12	25.931	31.654	45.752	1.000	16.34
ANISOU	83	CA	GLU	12	2703	1674	1831	-474	-889 1 0 3 3
ATOM	84	CB	GLU	12	26.527	31.477	47.158	1.000	16.09
ANISOU	84	CB	GLU	12	2440	1867	1808	-770	-820 1 0 5 8
ATOM	85	CG	GLU	12	26.633	32.802	47.915	1.000	18.90
ANISOU	85	CG	GLU	12	2717	2127	2335	-1216	-1090 7 8 8
ATOM	86	CD	GLU	12	27.115	32.657	49.342	1.000	21.17
ANISOU	86	CD	GLU	12	3300	2547	2198	-1182	-1053 7 2 4
ATOM	87	OE1	GLU	12	27.538	31.558	49.756	1.000	22.07
ANISOU	87	OE1	GLU	12	2722	3014	2650	-720	-1365 7 9 7
ATOM	88	OE2	GLU	12	27.068	33.679	50.059	1.000	29.26
ANISOU	88	OE2	GLU	12	5764	2634	2722	-1279	-1848 4 7 6
ATOM	89	C	GLU	12	25.997	30.402	44.882	1.000	17.16
ANISOU	89	C	GLU	12	2044	2319	2158	-624	-715 4 8 1
ATOM	90	O	GLU	12	26.879	30.317	44.032	1.000	18.88
ANISOU	90	O	GLU	12	3200	2388	1583	-1004	-306 8 9 9
ATOM	91	N	LEU	13	25.083	29.441	45.049	1.000	17.32
ANISOU	91	N	LEU	13	2176	2300	2104	-659	-386 9 4
ATOM	92	CA	LEU	13	25.082	28.252	44.189	1.000	14.00

- 93 -

ANISOU	92	CA	LEU	13	1734	1873	1713	-140	-170	4	9	8
ATOM	93	CB	LEU	13	24.003	27.248	44.620	1.000	15.3	7		
ANISOU	93	CB	LEU	13	2205	1838	1795	-375	-149	4	6	5
ATOM	94	CG	LEU	13	24.154	26.554	45.967	1.000	14.5	2		
ANISOU	94	CG	LEU	13	1913	1803	1799	-280	-204	4	4	2
ATOM	95	CD1	LEU	13	22.934	25.680	46.193	1.000	15.1	5		
ANISOU	95	CD1	LEU	13	2174	1817	1766	-433	185	1	7	5
ATOM	96	CD2	LEU	13	25.411	25.690	46.067	1.000	17.5	4		
ANISOU	96	CD2	LEU	13	2119	2043	2502	-38	-419	2	7	0
ATOM	97	C	LEU	13	24.876	28.626	42.725	1.000	16.5	4		
ANISOU	97	C	LEU	13	2510	2062	1710	-222	-93	5	6	5
ATOM	98	O	LEU	13	25.548	28.122	41.821	1.000	18.2	8		
ANISOU	98	O	LEU	13	2685	2514	1748	-687	75	2	5	9
ATOM	99	N	GLN	14	23.945	29.534	42.472	1.000	16.8	6		
ANISOU	99	N	GLN	14	1970	2337	2100	-557	-683	8	3	8
ATOM	100	CA	GLN	14	23.657	30.015	41.132	1.000	18.6	3		
ANISOU	100	CA	GLN	14	2761	2404	1915	-610	-802	5	6	8
ATOM	101	CB	GLN	14	22.421	30.923	41.130	1.000	19.3	9		
ANISOU	101	CB	GLN	14	3166	2176	2025	-392	-918	9	7	7
ATOM	102	CG	GLN	14	21.108	30.250	41.460	1.000	19.0	0		
ANISOU	102	CG	GLN	14	2879	2383	1957	-209	-725	4	6	0
ATOM	103	CD	GLN	14	19.974	31.227	41.766	1.000	18.8	3		
ANISOU	103	CD	GLN	14	3139	2118	1897	-6	-1229	4	9	4
ATOM	104	OE1	GLN	14	20.177	32.317	42.314	1.000	26.1	0		
ANISOU	104	OE1	GLN	14	3928	2407	3582	-98	-1172	-2	4	1
ATOM	105	NE2	GLN	14	18.745	30.823	41.411	1.000	20.9	4		
ANISOU	105	NE2	GLN	14	2900	2716	2340	-149	-840	4	5	4
ATOM	106	C	GLN	14	24.804	30.812	40.525	1.000	20.4	0		
ANISOU	106	C	GLN	14	3226	2458	2065	-795	-712	9	3	7
ATOM	107	O	GLN	14	24.812	30.951	39.311	1.000	30.4	8		
ANISOU	107	O	GLN	14	5089	4340	2152	-2337	-898	1	2	1
ATOM	108	N	GLN	15	25.734	31.309	41.329	1.000	20.3	5		
ANISOU	108	N	GLN	15	3252	2452	2030	-1067	-240	4	9	7
ATOM	109	CA	GLN	15	26.909	32.041	40.884	1.000	21.8	8		
ANISOU	109	CA	GLN	15	3184	3230	1901	-1152	-299	7	8	8
ATOM	110	CB	GLN	15	27.288	33.100	41.920	1.000	22.2	0		
ANISOU	110	CB	GLN	15	2720	3162	2551	-1131	-770	6	9	1
ATOM	111	CG	GLN	15	26.450	34.358	41.954	1.000	25.7	3		
ANISOU	111	CG	GLN	15	4496	2735	2545	-821	-233	1	2	6
ATOM	112	CD	GLN	15	26.325	35.021	43.306	1.000	35.7	6		
ANISOU	112	CD	GLN	15	6010	3945	3631	-643	-229	-1	3	5
ATOM	113	OE1	GLN	15	27.145	34.884	44.225	1.000	49.1	3		
ANISOU	113	OE1	GLN	15	8425	5866	4378	-2857	-2197	-5	6	4
ATOM	114	NE2	GLN	15	25.255	35.812	43.489	1.000	51.8	5		
ANISOU	114	NE2	GLN	15	7190	5567	6945	62	3066	1	0	7
ATOM	115	C	GLN	15	28.069	31.079	40.625	1.000	23.9	3		
ANISOU	115	C	GLN	15	3451	3513	2127	-990	145	8	8	4
ATOM	116	O	GLN	15	29.177	31.448	40.213	1.000	28.9	5		
ANISOU	116	O	GLN	15	3535	4619	2845	-899	510	1	2	2
ATOM	117	N	GLY	16	27.828	29.794	40.891	1.000	25.8	6		
ANISOU	117	N	GLY	16	4089	3282	2457	-889	-36	4	6	9
ATOM	118	CA	GLY	16	28.812	28.763	40.649	1.000	29.0	0		
ANISOU	118	CA	GLY	16	4785	3562	2671	-677	765	2	5	5
ATOM	119	C	GLY	16	29.741	28.546	41.814	1.000	25.4	5		
ANISOU	119	C	GLY	16	3427	3490	2754	-264	1422	6	7	3
ATOM	120	O	GLY	16	30.805	27.955	41.625	1.000	29.6	3		
ANISOU	120	O	GLY	16	3925	3267	4068	-66	1997	5	2	3
ATOM	121	N	LEU	17	29.387	28.979	43.015	1.000	22.5	0		
ANISOU	121	N	LEU	17	3266	2713	2569	-39	923	7	3	3
ATOM	122	CA	LEU	17	30.234	28.727	44.172	1.000	21.7	3		
ANISOU	122	CA	LEU	17	2299	2931	3025	-282	867	7	4	8

- 94 -

ATOM	123	CB	LEU	17	30.124	29.921	45.132	1.000	21.23
ANISOU	123	CB	LEU	17	2137	2858	3071	-620	669 7 1 1
ATOM	124	CG	LEU	17	30.354	31.274	44.431	1.000	26.12
ANISOU	124	CG	LEU	17	2708	2965	4253	-889	1342 9 3 1
ATOM	125	CD1	LEU	17	29.962	32.444	45.305	1.000	29.81
ANISOU	125	CD1	LEU	17	2515	2924	5885	-396	464 3 0 3
ATOM	126	CD2	LEU	17	31.808	31.350	43.974	1.000	32.84
ANISOU	126	CD2	LEU	17	2845	3703	5930	-281	1871 2 1 1 4
ATOM	127	C	LEU	17	29.886	27.456	44.936	1.000	19.36
ANISOU	127	C	LEU	17	2081	2819	2455	-239	545 5 8 0
ATOM	128	O	LEU	17	28.773	26.920	44.848	1.000	21.11
ANISOU	128	O	LEU	17	2284	3004	2734	-444	107 1 0 5 5
ATOM	129	N	HIS	18	30.838	26.952	45.706	1.000	21.02
ANISOU	129	N	HIS	18	2124	2752	3109	-314	193 4 9 1
ATOM	130	CA	HIS	18	30.678	25.814	46.615	1.000	18.11
ANISOU	130	CA	HIS	18	1569	2996	2315	-460	-28 3 6 1
ATOM	131	CB	HIS	18	29.655	26.149	47.702	1.000	21.25
ANISOU	131	CB	HIS	18	1731	3332	3010	-45	282 3 5 4
ATOM	132	CG	HIS	18	29.796	27.515	48.283	1.000	23.28
ANISOU	132	CG	HIS	18	2234	3612	2999	211	-46 - 2 0
ATOM	133	CD2	HIS	18	28.898	28.535	48.344	1.000	24.53
ANISOU	133	CD2	HIS	18	3112	3479	2728	532	41 4 4 0
ATOM	134	ND1	HIS	18	30.940	27.977	48.895	1.000	26.72
ANISOU	134	ND1	HIS	18	2938	4039	3173	-151	-569 3 8
ATOM	135	CE1	HIS	18	30.756	29.218	49.307	1.000	29.80
ANISOU	135	CE1	HIS	18	4476	3775	3071	-542	-562 2 3 7
ATOM	136	NE2	HIS	18	29.524	29.581	48.985	1.000	30.03
ANISOU	136	NE2	HIS	18	4752	3282	3377	216	-148 3 3 8
ATOM	137	C	HIS	18	30.266	24.528	45.917	1.000	18.57
ANISOU	137	C	HIS	18	1943	3084	2028	-951	30 5 9 0
ATOM	138	O	HIS	18	29.594	23.682	46.532	1.000	19.92
ANISOU	138	O	HIS	18	1949	3125	2493	-777	-87 9 9 5
ATOM	139	N	GLN	19	30.647	24.340	44.658	1.000	19.24
ANISOU	139	N	GLN	19	2329	2700	2282	-256	298 4 9 4
ATOM	140	CA	GLN	19	30.119	23.206	43.908	1.000	21.51
ANISOU	140	CA	GLN	19	3249	2431	2492	-228	597 3 1 8
ATOM	141	CB	GLN	19	30.446	23.307	42.406	1.000	22.89
ANISOU	141	CB	GLN	19	3231	3058	2408	-148	463 2 4 4
ATOM	142	CG	GLN	19	29.738	24.453	41.698	1.000	25.83
ANISOU	142	CG	GLN	19	3445	3712	2658	-384	-407 5 6 8
ATOM	143	CD	GLN	19	28.223	24.470	41.747	1.000	31.56
ANISOU	143	CD	GLN	19	3439	4722	3832	-252	-988 3 5 7
ATOM	144	OE1	GLN	19	27.521	23.640	41.153	1.000	38.51
ANISOU	144	OE1	GLN	19	3869	3649	7115	377	-3045 6 8 6
ATOM	145	NE2	GLN	19	27.621	25.433	42.475	1.000	33.32
ANISOU	145	NE2	GLN	19	3303	5695	3663	647	-1109 4 4 9
ATOM	146	C	GLN	19	30.578	21.873	44.485	1.000	20.32
ANISOU	146	C	GLN	19	2224	2710	2785	-60	514 3 9 4
ATOM	147	O	GLN	19	29.806	20.900	44.473	1.000	19.08
ANISOU	147	O	GLN	19	1888	2451	2910	221	257 7 4 3
ATOM	148	N	ASP	20	31.800	21.761	44.999	1.000	24.09
ANISOU	148	N	ASP	20	3001	3507	2645	-773	-507 4 1 5
ATOM	149	CA	ASP	20	32.268	20.498	45.553	1.000	21.82
ANISOU	149	CA	ASP	20	1707	3811	2774	-327	-58 3 5 7
ATOM	150	CB	ASP	20	33.780	20.527	45.779	1.000	26.34
ANISOU	150	CB	ASP	20	1594	4552	3863	-962	236 4 9 0
ATOM	151	CG	ASP	20	34.596	20.517	44.503	1.000	34.45
ANISOU	151	CG	ASP	20	2531	5859	4701	-1208	1213 - 2 8 0
ATOM	152	OD1	ASP	20	34.177	19.982	43.457	1.000	33.11
ANISOU	152	OD1	ASP	20	3768	4173	4640	-311	1233 - 3 7 5
ATOM	153	OD2	ASP	20	35.725	21.056	44.532	1.000	49.71

- 95 -

ANISOU	153	OD2	ASP	20	3445	9922	5519	-3116	1710	5	3
ATOM	154	C	ASP	20	31.538	20.179	46.862	1.000	21.03		
ANISOU	154	C	ASP	20	1876	2702	3412	-231	616	3	8 8
ATOM	155	O	ASP	20	31.118	19.038	47.075	1.000	20.80		
ANISOU	155	O	ASP	20	1162	2583	4157	-72	-139	5	5 0
ATOM	156	N	GLU	21	31.359	21.177	47.729	1.000	17.88		
ANISOU	156	N	GLU	21	1218	2751	2824	-263	-148	5	1 1
ATOM	157	CA	GLU	21	30.599	20.999	48.965	1.000	16.80		
ANISOU	157	CA	GLU	21	1128	2173	3083	-96	46	3	9 4
ATOM	158	CB	GLU	21	30.654	22.304	49.781	1.000	20.23		
ANISOU	158	CB	GLU	21	1366	2620	3701	5	-262	-2	1 0
ATOM	159	CG	GLU	21	32.040	22.669	50.307	1.000	24.60		
ANISOU	159	CG	GLU	21	1660	3325	4359	-221	-654	-3	0 1
ATOM	160	CD	GLU	21	32.860	23.565	49.402	1.000	28.46		
ANISOU	160	CD	GLU	21	1191	4348	5275	-498	-1597	1	1 2 5
ATOM	161	OE1	GLU	21	33.751	24.294	49.919	1.000	31.17		
ANISOU	161	OE1	GLU	21	2360	4428	5057	-1039	-1094	3	4 9
ATOM	162	OE2	GLU	21	32.664	23.590	48.171	1.000	31.16		
ANISOU	162	OE2	GLU	21	2734	3901	5203	-1519	-1565	1	1 2 3
ATOM	163	C	GLU	21	29.159	20.594	48.689	1.000	16.44		
ANISOU	163	C	GLU	21	1271	2295	2679	-165	-53	4	3 0
ATOM	164	O	GLU	21	28.599	19.700	49.329	1.000	14.30		
ANISOU	164	O	GLU	21	1271	2257	1907	-417	-301	3	6
ATOM	165	N	PHE	22	28.548	21.257	47.708	1.000	16.14		
ANISOU	165	N	PHE	22	1440	2441	2253	-316	-28	3	2 8
ATOM	166	CA	PHE	22	27.155	20.947	47.327	1.000	15.36		
ANISOU	166	CA	PHE	22	1530	2012	2294	-262	-173	2	8 1
ATOM	167	CB	PHE	22	26.612	21.967	46.343	1.000	15.43		
ANISOU	167	CB	PHE	22	1863	2056	1944	-316	-247	1	8 4
ATOM	168	CG	PHE	22	25.119	21.932	46.077	1.000	15.59		
ANISOU	168	CG	PHE	22	1822	2141	1962	-299	-170	5	6 1
ATOM	169	CD1	PHE	22	24.218	21.987	47.129	1.000	17.03		
ANISOU	169	CD1	PHE	22	1923	2605	1943	-410	-162	-4	0
ATOM	170	CD2	PHE	22	24.606	21.856	44.797	1.000	14.84		
ANISOU	170	CD2	PHE	22	1541	2083	2013	51	-94	-1	5 5
ATOM	171	CE1	PHE	22	22.861	21.938	46.906	1.000	15.96		
ANISOU	171	CE1	PHE	22	1844	1805	2414	-159	-64	1	7 6
ATOM	172	CE2	PHE	22	23.243	21.797	44.551	1.000	15.81		
ANISOU	172	CE2	PHE	22	1600	1993	2416	-261	-190	-1	7 6
ATOM	173	CZ	PHE	22	22.360	21.853	45.612	1.000	14.18		
ANISOU	173	CZ	PHE	22	1427	1430	2531	-105	-164	3	2 5
ATOM	174	C	PHE	22	27.049	19.515	46.792	1.000	16.23		
ANISOU	174	C	PHE	22	1325	2042	2797	-110	164	1	0 2
ATOM	175	O	PHE	22	26.183	18.751	47.229	1.000	13.24		
ANISOU	175	O	PHE	22	1411	1743	1876	105	-194	3	9 1
ATOM	176	N	ARG	23	27.888	19.097	45.853	1.000	15.45		
ANISOU	176	N	ARG	23	1585	2313	1971	-167	-80	2	8 9
ATOM	177	CA	ARG	23	27.865	17.746	45.325	1.000	15.49		
ANISOU	177	CA	ARG	23	809 2443	2634	50	-41	-2	2	
ATOM	178	CB	ARG	23	28.928	17.539	44.248	1.000	17.81		
ANISOU	178	CB	ARG	23	966 3142	2658	-128	43	-1	6 7	
ATOM	179	CG	ARG	23	28.470	17.928	42.860	1.000	25.86		
ANISOU	179	CG	ARG	23	2719	4636	2470	-758	-176	-4	9
ATOM	180	CD	ARG	23	29.485	17.370	41.867	1.000	34.68		
ANISOU	180	CD	ARG	23	5148	4847	3183	-1532	1634	-5	4 8
ATOM	181	NE	ARG	23	30.660	18.253	41.877	1.000	31.13		
ANISOU	181	NE	ARG	23	2799	4194	4836	305	747	6	6
ATOM	182	CZ	ARG	23	30.703	19.424	41.244	1.000	34.24		
ANISOU	182	CZ	ARG	23	2749	4844	5418	-757	239	7	6 4
ATOM	183	NH1	ARG	23	29.647	19.856	40.551	1.000	28.06		
ANISOU	183	NH1	ARG	23	2714	3685	4263	-721	555	1	8 1

- 96 -

ATOM	184	NH2	ARG	23	31.830	20.114	41.340	1.000	36.08		
ANISOU	184	NH2	ARG	23	2261	5328	6121	-562	776	-86	
ATOM	185	C	ARG	23	28.045	16.713	46.420	1.000	15.06		
ANISOU	185	C	ARG	23	1071	2061	2589	167	-32	-234	
ATOM	186	O	ARG	23	27.335	15.687	46.410	1.000	16.28		
ANISOU	186	O	ARG	23	1443	2244	2497	-118	-71	-277	
ATOM	187	N	ARG	24	28.952	16.988	47.353	1.000	15.27		
ANISOU	187	N	ARG	24	1024	2156	2623	-52	-21	29	
ATOM	188	CA	ARG	24	29.193	16.003	48.430	1.000	17.70		
ANISOU	188	CA	ARG	24	1443	2589	2693	275	-2	215	
ATOM	189	CB	ARG	24	30.466	16.422	49.148	1.000	21.11		
ANISOU	189	CB	ARG	24	1244	3486	3289	484	-257	384	
ATOM	190	CG	ARG	24	31.787	16.217	48.429	1.000	30.46		
ANISOU	190	CG	ARG	24	1438	5078	5057	426	441	308	
ATOM	191	CD	ARG	24	32.979	16.537	49.330	1.000	33.50		
ANISOU	191	CD	ARG	24	1163	5831	5736	208	370	458	
ATOM	192	NE	ARG	24	33.636	17.804	49.071	1.000	51.46		
ANISOU	192	NE	ARG	24	5800	7316	6437	-2596	-1688	1165	
ATOM	193	CZ	ARG	24	33.973	18.776	49.903	1.000	46.72		
ANISOU	193	CZ	ARG	24	4738	6888	6124	-1719	-1822	1316	
ATOM	194	NH1	ARG	24	33.731	18.728	51.213	1.000	44.24		
ANISOU	194	NH1	ARG	24	2650	6998	7160	-392	1001	84	
ATOM	195	NH2	ARG	24	34.579	19.871	49.448	1.000	42.82		
ANISOU	195	NH2	ARG	24	5339	4428	6503	513	-991	1216	
ATOM	196	C	ARG	24	27.972	15.887	49.334	1.000	17.16		
ANISOU	196	C	ARG	24	1549	2071	2900	129	140	295	
ATOM	197	O	ARG	24	27.536	14.779	49.713	1.000	15.38		
ANISOU	197	O	ARG	24	1706	1890	2247	72	-388	104	
ATOM	198	N	CYS	25	27.355	17.011	49.696	1.000	12.91		
ANISOU	198	N	CYS	25	9071824	2176	-254	-386	151		
ATOM	199	CA	CYS	25	26.105	17.040	50.454	1.000	12.45		
ANISOU	199	CA	CYS	25	9421838	1949	-178	-480	81		
ATOM	200	CB	CYS	25	25.660	18.491	50.697	1.000	11.67		
ANISOU	200	CB	CYS	25	1150	1759	1527	-136	-604	184	
ATOM	201	SG	CYS	25	23.973	18.580	51.425	1.000	14.90		
ANISOU	201	SG	CYS	25	1465	1593	2602	-164	-26	-18	
ATOM	202	C	CYS	25	25.001	16.225	49.769	1.000	11.67		
ANISOU	202	C	CYS	25	8931897	1645	-283	-64	-86		
ATOM	203	O	CYS	25	24.360	15.377	50.390	1.000	12.73		
ANISOU	203	O	CYS	25	1347	1426	2064	-233	-196	123	
ATOM	204	N	LEU	26	24.798	16.461	48.470	1.000	11.70		
ANISOU	204	N	LEU	26	1102	1530	1814	-128	-390	1	
ATOM	205	CA	LEU	26	23.766	15.716	47.735	1.000	11.11		
ANISOU	205	CA	LEU	26	1190	1476	1556	-238	-79	-194	
ATOM	206	CB	LEU	26	23.674	16.198	46.285	1.000	11.54		
ANISOU	206	CB	LEU	26	1345	1522	1518	-75	-84	-202	
ATOM	207	CG	LEU	26	23.242	17.638	46.019	1.000	12.42		
ANISOU	207	CG	LEU	26	1199	1542	1978	-153	-167	-40	
ATOM	208	CD1	LEU	26	23.414	17.993	44.539	1.000	14.77		
ANISOU	208	CD1	LEU	26	1428	1916	2270	43	131	401	
ATOM	209	CD2	LEU	26	21.814	17.885	46.466	1.000	14.45		
ANISOU	209	CD2	LEU	26	1384	2061	2047	264	-32	321	
ATOM	210	C	LEU	26	23.979	14.209	47.780	1.000	12.93		
ANISOU	210	C	LEU	26	1360	1542	2011	-121	-486	-107	
ATOM	211	O	LEU	26	23.011	13.461	48.008	1.000	13.78		
ANISOU	211	O	LEU	26	1660	1450	2125	-305	-426	-51	
ATOM	212	N	ARG	27	25.196	13.721	47.576	1.000	14.09		
ANISOU	212	N	ARG	27	1518	1729	2108	151	-530	-105	
ATOM	213	CA	ARG	27	25.491	12.283	47.574	1.000	15.39		
ANISOU	213	CA	ARG	27	2260	1690	1897	186	141	-354	
ATOM	214	CB	ARG	27	26.846	12.122	46.900	1.000	17.04		

- 97 -

ANISOU	214	CB	ARG	27	2259	2356	1861	517	49	- 2 4 8
ATOM	215	CG	ARG	27	27.502	10.780	46.801	1.000	25.08	
ANISOU	215	CG	ARG	27	3110	2837	3583	1105	606	- 3 9 9
ATOM	216	CD	ARG	27	28.995	10.992	46.457	1.000	30.32	
ANISOU	216	CD	ARG	27	2976	3836	4710	1190	720	- 1 3 8 1
ATOM	217	NE	ARG	27	29.818	11.407	47.581	1.000	36.51	
ANISOU	217	NE	ARG	27	3633	4937	5301	121	391	- 1 4 2 9
ATOM	218	CZ	ARG	27	30.988	12.019	47.560	1.000	38.07	
ANISOU	218	CZ	ARG	27	3334	5192	5941	364	661	- 1 7 7 6
ATOM	219	NH1	ARG	27	31.565	12.340	46.401	1.000	48.56	
ANISOU	219	NH1	ARG	27	4482	7688	6280	-1305	736	- 1 3 2 6
ATOM	220	NH2	ARG	27	31.606	12.328	48.701	1.000	40.23	
ANISOU	220	NH2	ARG	27	2891	6127	6266	457	717	- 2 4 6 3
ATOM	221	C	ARG	27	25.479	11.630	48.949	1.000	14.66	
ANISOU	221	C	ARG	27	1720	1617	2233	135	-33	- 4 2
ATOM	222	O	ARG	27	24.968	10.499	49.072	1.000	17.44	
ANISOU	222	O	ARG	27	1981	1533	3114	98	-394	1 5 5
ATOM	223	N	ASP	28	26.031	12.308	49.973	1.000	13.72	
ANISOU	223	N	ASP	28	1703	1366	2146	317	-327	3 1 9
ATOM	224	CA	ASP	28	26.227	11.701	51.277	1.000	15.33	
ANISOU	224	CA	ASP	28	1886	1704	2234	538	-247	3 9 1
ATOM	225	CB	ASP	28	27.541	12.280	51.842	1.000	18.31	
ANISOU	225	CB	ASP	28	2092	2709	2155	186	-465	5 4 4
ATOM	226	CG	ASP	28	28.785	11.875	51.083	1.000	23.06	
ANISOU	226	CG	ASP	28	2002	3583	3176	-96	-50	4 7 8
ATOM	227	OD1	ASP	28	28.741	10.904	50.290	1.000	25.09	
ANISOU	227	OD1	ASP	28	2515	2855	4163	830	406	4 4 0
ATOM	228	OD2	ASP	28	29.831	12.528	51.283	1.000	30.05	
ANISOU	228	OD2	ASP	28	1919	4262	5236	-216	-695	1 0 5 8
ATOM	229	C	ASP	28	25.092	11.910	52.267	1.000	14.90	
ANISOU	229	C	ASP	28	2071	1435	2154	411	-203	2 1 7
ATOM	230	O	ASP	28	24.967	11.093	53.200	1.000	14.50	
ANISOU	230	O	ASP	28	1878	1501	2132	444	-265	1 7 9
ATOM	231	N	LYS	29	24.317	12.975	52.096	1.000	12.90	
ANISOU	231	N	LYS	29	1487	1290	2126	77	-276	1 3 6
ATOM	232	CA	LYS	29	23.265	13.368	53.029	1.000	12.95	
ANISOU	232	CA	LYS	29	1369	1649	1904	8	-390	1 4
ATOM	233	CB	LYS	29	23.699	14.653	53.763	1.000	12.71	
ANISOU	233	CB	LYS	29	1105	1581	2145	209	-359	- 3 0
ATOM	234	CG	LYS	29	25.016	14.504	54.518	1.000	16.11	
ANISOU	234	CG	LYS	29	1413	1998	2711	21	-818	- 1 6 1
ATOM	235	CD	LYS	29	25.449	15.727	55.309	1.000	18.24	
ANISOU	235	CD	LYS	29	2500	1989	2442	-47	-1140	- 1 4
ATOM	236	CE	LYS	29	26.789	15.445	56.002	1.000	19.36	
ANISOU	236	CE	LYS	29	2038	3171	2148	-90	-822	- 7 2 5
ATOM	237	NZ	LYS	29	27.515	16.696	56.351	1.000	26.61	
ANISOU	237	NZ	LYS	29	2592	3146	4373	-309	-1571	- 3 5 3
ATOM	238	C	LYS	29	21.888	13.550	52.386	1.000	11.62	
ANISOU	238	C	LYS	29	1432	1153	1831	52	-290	2 4
ATOM	239	O	LYS	29	20.877	13.028	52.880	1.000	12.57	
ANISOU	239	O	LYS	29	1426	1556	1792	-97	-282	1 0 0
ATOM	240	N	GLY	30	21.779	14.280	51.284	1.000	11.98	
ANISOU	240	N	GLY	30	1359	1454	1741	-5	-310	7 8
ATOM	241	CA	GLY	30	20.510	14.478	50.562	1.000	10.93	
ANISOU	241	CA	GLY	30	1192	1497	1465	-158	-116	- 1 8
ATOM	242	C	GLY	30	19.544	15.433	51.242	1.000	11.15	
ANISOU	242	C	GLY	30	1137	1143	1955	-260	-154	- 1 3 1
ATOM	243	O	GLY	30	18.337	15.374	50.963	1.000	11.26	
ANISOU	243	O	GLY	30	1247	1082	1949	-56	-419	1 0 4
ATOM	244	N	LEU	31	20.064	16.278	52.129	1.000	10.54	
ANISOU	244	N	LEU	31	1292	894	1821	-98	-367	8 9

- 98 -

ATOM	245	CA	LEU	31	19.272	17.324	52.803	1.000	11.07
ANISOU	245	CA	LEU	31	1345	1111	1752	46	-520 - 3 3
ATOM	246	CB	LEU	31	18.465	16.777	53.975	1.000	14.44
ANISOU	246	CB	LEU	31	1753	1671	2062	-284	-80 - 17 8
ATOM	247	CG	LEU	31	19.113	16.629	55.333	1.000	17.74
ANISOU	247	CG	LEU	31	2456	2220	2064	-172	-115 4 9 9
ATOM	248	CD1	LEU	31	18.220	15.978	56.371	1.000	26.19
ANISOU	248	CD1	LEU	31	2716	4691	2543	-1224	-213 10 1 6
ATOM	249	CD2	LEU	31	20.388	15.821	55.182	1.000	22.77
ANISOU	249	CD2	LEU	31	3121	2633	2899	650	-18 1 4 8 7
ATOM	250	C	LEU	31	20.176	18.498	53.195	1.000	10.95
ANISOU	250	C	LEU	31	1041	1129	1989	180	-318 - 2 2 3
ATOM	251	O	LEU	31	21.376	18.314	53.424	1.000	10.89
ANISOU	251	O	LEU	31	1015	1171	1952	69	-160 2 0 4
ATOM	252	N	PHE	32	19.570	19.688	53.219	1.000	11.42
ANISOU	252	N	PHE	32	1134	995 2211	75	-273	6 5
ATOM	253	CA	PHE	32	20.280	20.916	53.545	1.000	10.33
ANISOU	253	CA	PHE	32	1071	1152	1703	-57	-288 - 3 3
ATOM	254	CB	PHE	32	21.244	21.307	52.422	1.000	12.25
ANISOU	254	CB	PHE	32	1054	1729	1872	-113	-173 - 5
ATOM	255	CG	PHE	32	20.624	21.346	51.041	1.000	11.94
ANISOU	255	CG	PHE	32	1158	1572	1809	-281	-148 1 2 2
ATOM	256	CD1	PHE	32	20.522	20.188	50.270	1.000	11.12
ANISOU	256	CD1	PHE	32	1070	1308	1846	-182	-458 3 1 8
ATOM	257	CD2	PHE	32	20.145	22.528	50.513	1.000	12.14
ANISOU	257	CD2	PHE	32	1618	1353	1639	-300	-185 - 4 7
ATOM	258	CE1	PHE	32	19.943	20.212	49.015	1.000	12.00
ANISOU	258	CE1	PHE	32	1342	1377	1840	-301	-468 3 3 2
ATOM	259	CE2	PHE	32	19.553	22.534	49.266	1.000	12.79
ANISOU	259	CE2	PHE	32	1858	1543	1457	-86	-34 2 8
ATOM	260	CZ	PHE	32	19.416	21.376	48.503	1.000	11.50
ANISOU	260	CZ	PHE	32	1623	1414	1331	-76	-272 2 1 7
ATOM	261	C	PHE	32	19.310	22.071	53.762	1.000	9.82
ANISOU	261	C	PHE	32	1015	1042	1674	-120	-367 - 7 7
ATOM	262	O	PHE	32	18.165	21.990	53.285	1.000	11.29
ANISOU	262	O	PHE	32	1097	1286	1906	-95	-495 - 7 7
ATOM	263	N	TYR	33	19.736	23.099	54.493	1.000	12.68
ANISOU	263	N	TYR	33	1606	1053	2158	-57	-766 - 15 9
ATOM	264	CA	TYR	33	18.945	24.335	54.607	1.000	10.64
ANISOU	264	CA	TYR	33	1491	1173	1380	-77	-97 - 13 2
ATOM	265	CB	TYR	33	19.141	25.022	55.955	1.000	10.85
ANISOU	265	CB	TYR	33	1019	1725	1379	-260	-224 - 1 6 4
ATOM	266	CG	TYR	33	18.545	24.331	57.156	1.000	10.71
ANISOU	266	CG	TYR	33	1173	1552	1342	-45	-230 - 11 7
ATOM	267	CD1	TYR	33	17.266	24.643	57.619	1.000	11.64
ANISOU	267	CD1	TYR	33	1385	1441	1596	-68	83 - 9 4
ATOM	268	CE1	TYR	33	16.694	24.023	58.719	1.000	13.60
ANISOU	268	CE1	TYR	33	1879	1483	1804	-147	339 - 2 6
ATOM	269	CD2	TYR	33	19.273	23.364	57.853	1.000	14.04
ANISOU	269	CD2	TYR	33	1604	2040	1689	132	-509 1 2 7
ATOM	270	CE2	TYR	33	18.711	22.752	58.964	1.000	15.75
ANISOU	270	CE2	TYR	33	1872	2227	1886	-187	-701 4 3 3
ATOM	271	CZ	TYR	33	17.438	23.078	59.387	1.000	16.02
ANISOU	271	CZ	TYR	33	2205	1939	1942	-332	-154 3 0 0
ATOM	272	OH	TYR	33	16.919	22.454	60.504	1.000	19.95
ANISOU	272	OH	TYR	33	3412	2154	2015	-60	278 4 0 0
ATOM	273	C	TYR	33	19.357	25.253	53.452	1.000	10.92
ANISOU	273	C	TYR	33	1249	1448	1453	-125	-271 1 4 9
ATOM	274	O	TYR	33	20.514	25.192	53.006	1.000	11.50
ANISOU	274	O	TYR	33	1204	1375	1791	-98	-270 2 8 1
ATOM	275	N	LEU	34	18.399	26.049	53.000	1.000	11.28

- 99 -

ANISOU	275	N	LEU	34	1159	1265	1862	-210	-149	1	2	1
ATOM	276	CA	LEU	34	18.577	26.942	51.864	1.000	12.99			
ANISOU	276	CA	LEU	34	1565	1444	1926	81	-478	2	7	4
ATOM	277	CB	LEU	34	17.757	26.420	50.682	1.000	13.96			
ANISOU	277	CB	LEU	34	2007	1301	1995	-430	-459	3	2	1
ATOM	278	CG	LEU	34	17.990	27.112	49.334	1.000	13.81			
ANISOU	278	CG	LEU	34	2085	1322	1839	-331	-365	1	9	8
ATOM	279	CD1	LEU	34	19.308	26.691	48.704	1.000	15.94			
ANISOU	279	CD1	LEU	34	2123	1793	2140	-10	-313	6	0	7
ATOM	280	CD2	LEU	34	16.818	26.799	48.411	1.000	16.36			
ANISOU	280	CD2	LEU	34	2186	1837	2193	122	-721	1	3	4
ATOM	281	C	LEU	34	18.195	28.361	52.241	1.000	13.03			
ANISOU	281	C	LEU	34	1676	1418	1857	31	-643	2	1	8
ATOM	282	O	LEU	34	17.055	28.647	52.595	1.000	13.99			
ANISOU	282	O	LEU	34	1690	1281	2344	140	-714	8	5	
ATOM	283	N	THR	35	19.148	29.283	52.175	1.000	15.03			
ANISOU	283	N	THR	35	1837	1584	2288	-118	-625	-	3	
ATOM	284	CA	THR	35	18.918	30.704	52.369	1.000	14.80			
ANISOU	284	CA	THR	35	1866	1560	2196	-169	-175	-	1	4
ATOM	285	CB	THR	35	20.013	31.366	53.232	1.000	15.65			
ANISOU	285	CB	THR	35	2025	1719	2202	-149	-204	-	2	8
ATOM	286	OG1	THR	35	21.276	31.115	52.601	1.000	18.81			
ANISOU	286	OG1	THR	35	1885	2679	2583	-279	-229	-	7	2
ATOM	287	CG2	THR	35	20.138	30.811	54.622	1.000	18.84			
ANISOU	287	CG2	THR	35	2523	2207	2427	-850	-510	1	5	5
ATOM	288	C	THR	35	18.915	31.456	51.043	1.000	15.07			
ANISOU	288	C	THR	35	1904	1473	2348	-57	-283	-	7	0
ATOM	289	O	THR	35	19.209	30.909	49.973	1.000	15.00			
ANISOU	289	O	THR	35	2034	1520	2145	-215	-372	8	9	
ATOM	290	N	ASP	36	18.564	32.739	51.086	1.000	17.46			
ANISOU	290	N	ASP	36	2302	1366	2968	-209	-766	-	1	2
ATOM	291	CA	ASP	36	18.618	33.606	49.924	1.000	17.91			
ANISOU	291	CA	ASP	36	2150	1592	3063	112	-660	8	6	
ATOM	292	CB	ASP	36	20.063	33.845	49.471	1.000	17.91			
ANISOU	292	CB	ASP	36	2153	1584	3067	84	-587	-	4	2
ATOM	293	CG	ASP	36	20.948	34.545	50.469	1.000	19.23			
ANISOU	293	CG	ASP	36	2575	2160	2571	-642	-324	1	8	1
ATOM	294	OD1	ASP	36	20.426	35.304	51.325	1.000	24.17			
ANISOU	294	OD1	ASP	36	2843	3055	3284	152	-1013	-	6	5
ATOM	295	OD2	ASP	36	22.199	34.355	50.412	1.000	21.00			
ANISOU	295	OD2	ASP	36	2637	2571	2772	-382	-834	-	3	9
ATOM	296	C	ASP	36	17.783	33.038	48.784	1.000	18.20			
ANISOU	296	C	ASP	36	2402	1736	2779	-446	-390	1	9	1
ATOM	297	O	ASP	36	18.222	33.063	47.629	1.000	18.98			
ANISOU	297	O	ASP	36	2127	2022	3062	-464	-60	-	2	5
ATOM	298	N	CYS	37	16.593	32.547	49.077	1.000	17.22			
ANISOU	298	N	CYS	37	1873	2190	2479	63	-350	-	1	
ATOM	299	CA	CYS	37	15.730	31.945	48.043	1.000	15.98			
ANISOU	299	CA	CYS	37	1997	1590	2485	-81	-65	-	1	8
ATOM	300	CB	CYS	37	15.621	30.423	48.252	1.000	18.87			
ANISOU	300	CB	CYS	37	2112	1790	3268	-114	-405	5	7	0
ATOM	301	SG	CYS	37	14.753	29.917	49.759	1.000	19.42			
ANISOU	301	SG	CYS	37	2532	1683	3164	-74	-230	3	2	2
ATOM	302	C	CYS	37	14.349	32.580	47.958	1.000	16.12			
ANISOU	302	C	CYS	37	1992	1669	2465	-175	-504	1	6	
ATOM	303	O	CYS	37	13.483	32.032	47.253	1.000	20.60			
ANISOU	303	O	CYS	37	2761	1769	3296	-241	-1333	5	1	
ATOM	304	N	GLY	38	14.125	33.714	48.617	1.000	17.89			
ANISOU	304	N	GLY	38	1847	1572	3381	209	-898	-	1	1
ATOM	305	CA	GLY	38	12.850	34.404	48.587	1.000	18.16			
ANISOU	305	CA	GLY	38	1608	2126	3164	141	-999	-	6	

- 100 -

ATOM	306	C	GLY	38	11.843	33.864	49.589	1.000	21.98
ANISOU	306	C	GLY	38	2598	2574	3180	262	-97 - 4 5 5
ATOM	307	O	GLY	38	10.677	34.273	49.499	1.000	22.75
ANISOU	307	O	GLY	38	2542	3027	3073	241	79 - 9 7
ATOM	308	N	LEU	39	12.241	32.982	50.501	1.000	21.93
ANISOU	308	N	LEU	39	2112	3318	2903	-65	-102 - 1 5 4
ATOM	309	CA	LEU	39	11.443	32.357	51.545	1.000	26.16
ANISOU	309	CA	LEU	39	3141	3610	3188	-1071	162 - 4 0 0
ATOM	310	CB	LEU	39	11.220	30.868	51.277	1.000	28.13
ANISOU	310	CB	LEU	39	2980	3192	4516	-352	-848 2 5 8
ATOM	311	CG	LEU	39	10.296	30.434	50.157	1.000	27.39
ANISOU	311	CG	LEU	39	3352	2591	4463	541	-637 - 1 0 5 2
ATOM	312	CD1	LEU	39	10.472	28.940	49.910	1.000	28.66
ANISOU	312	CD1	LEU	39	3375	2293	5221	581	-150 - 1 9 0
ATOM	313	CD2	LEU	39	8.838	30.768	50.478	1.000	30.62
ANISOU	313	CD2	LEU	39	3155	2985	5496	1275	-1485 - 2 0 8
ATOM	314	C	LEU	39	12.060	32.430	52.949	1.000	26.26
ANISOU	314	C	LEU	39	2868	3969	3143	-796	170 3 3 5
ATOM	315	O	LEU	39	13.105	31.861	53.266	1.000	35.57
ANISOU	315	O	LEU	39	4990	4057	4470	804	-630 3 2 0
ATOM	316	N	THR	40	11.388	33.136	53.827	1.000	26.61
ANISOU	316	N	THR	40	3425	3883	2803	-703	-191 1 0 2
ATOM	317	CA	THR	40	11.676	33.329	55.228	1.000	22.95
ANISOU	317	CA	THR	40	1972	3864	2886	4	-608 5 1 8
ATOM	318	C	THR	40	10.380	33.424	56.031	1.000	27.03
ANISOU	318	C	THR	40	2331	4900	3040	-690	-220 - 3
ATOM	319	O	THR	40	9.254	33.316	55.537	1.000	25.98
ANISOU	319	O	THR	40	2148	4860	2864	-546	36 - 7 2 0
ATOM	320	CB	THR	40	12.476	34.624	55.456	1.000	27.16
ANISOU	320	CB	THR	40	2646	4799	2874	-932	-391 1 4 8
ATOM	321	OG1	THR	40	11.639	35.687	54.986	1.000	36.24
ANISOU	321	OG1	THR	40	5158	3872	4740	-472	-136 6 6 0
ATOM	322	CG2	THR	40	13.771	34.669	54.659	1.000	34.29
ANISOU	322	CG2	THR	40	5268	3289	4470	-1303	2206 4 2 9
ATOM	323	N	ASP	41	10.524	33.635	57.346	1.000	28.20
ANISOU	323	N	ASP	41	2270	5223	3223	-711	-317 - 4 7 9
ATOM	324	CA	ASP	41	9.324	33.604	58.191	1.000	25.10
ANISOU	324	CA	ASP	41	1935	4633	2968	13	-551 - 5 0 5
ATOM	325	C	ASP	41	8.418	34.785	57.896	1.000	24.69
ANISOU	325	C	ASP	41	2686	3839	2855	-446	-749 - 2 4 1
ATOM	326	O	ASP	41	7.219	34.846	58.163	1.000	24.79
ANISOU	326	O	ASP	41	2757	2721	3941	174	-584 - 1 4 1
ATOM	327	CB	ASP	41	9.728	33.549	59.678	1.000	28.21
ANISOU	327	CB	ASP	41	2221	5503	2995	892	-594 - 5 5 5
ATOM	328	CG	ASP	41	9.892	32.129	60.180	1.000	42.46
ANISOU	328	CG	ASP	41	6437	5911	3784	-1196	-1257 8 2 6
ATOM	329	OD1	ASP	41	9.705	31.161	59.401	1.000	55.96
ANISOU	329	OD1	ASP	41	12184	5138	3940	-2654	-82 1 2 4 9
ATOM	330	OD2	ASP	41	10.214	31.951	61.383	1.000	61.55
ANISOU	330	OD2	ASP	41	10370	7470	5548	-4396	-4720 2 3 0 9
ATOM	331	N	THR	42	8.991	35.807	57.305	1.000	29.30
ANISOU	331	N	THR	42	3761	4531	2839	-1404	-1089 - 7 2
ATOM	332	CA	THR	42	8.255	36.976	56.863	1.000	33.69
ANISOU	332	CA	THR	42	4852	3472	4475	-1524	-819 - 1 2 7
ATOM	333	C	THR	42	7.199	36.598	55.834	1.000	29.14
ANISOU	333	C	THR	42	3354	3051	4667	204	-648 - 2 7 7
ATOM	334	O	THR	42	6.026	36.969	55.844	1.000	36.90
ANISOU	334	O	THR	42	3578	2980	7462	603	-176 6 4 3
ATOM	335	CB	THR	42	9.282	37.967	56.281	1.000	40.80
ANISOU	335	CB	THR	42	5831	4318	5354	-2254	-450 3 7
ATOM	336	OG1	THR	42	10.288	38.317	57.263	1.000	46.30

- 101 -

ANISOU	336	OG1	THR	42	6998	3682	6912	-3163	-1478	1 7 7
ATOM	337	CG2	THR	42	8.582	39.253	55.872	1.000	45.59	
ANISOU	337	CG2	THR	42	9083	3877	4363	-2166	-1048	2 3 8
ATOM	338	N	GLU	43	7.573	35.773	54.862	1.000	31.74	
ANISOU	338	N	GLU	43	3380	4360	4319	-673	-223	-7 8 2
ATOM	339	CA	GLU	43	6.647	35.355	53.810	1.000	35.40	
ANISOU	339	CA	GLU	43	4856	4683	3913	-1510	-860	3 2 9
ATOM	340	C	GLU	43	5.643	34.324	54.330	1.000	28.03	
ANISOU	340	C	GLU	43	2988	3297	4363	-41	-919	1 6 8
ATOM	341	O	GLU	43	4.560	34.138	53.764	1.000	38.18	
ANISOU	341	O	GLU	43	3818	2970	7717	-66	-2774	1 4 6 9
ATOM	342	CB	GLU	43	7.423	34.811	52.608	1.000	38.89	
ANISOU	342	CB	GLU	43	4464	6532	3779	-2546	-860	-3 9 3
ATOM	343	CG	GLU	43	8.462	35.745	52.010	1.000	46.47	
ANISOU	343	CG	GLU	43	5175	7105	5377	-2936	-92	-2 8 9
ATOM	344	CD	GLU	43	9.750	35.764	52.826	1.000	46.40	
ANISOU	344	CD	GLU	43	4506	7977	5145	-3155	548	-1 2 1 0
ATOM	345	OE1	GLU	43	9.775	36.447	53.880	1.000	55.20	
ANISOU	345	OE1	GLU	43	8741	7607	4627	-2062	-1002	-6 6 9
ATOM	346	OE2	GLU	43	10.706	35.080	52.433	1.000	56.77	
ANISOU	346	OE2	GLU	43	4592	8930	8050	-2652	939	-1 2 5 8
ATOM	347	N	LEU	44	5.980	33.645	55.426	1.000	22.72	
ANISOU	347	N	LEU	44	2508	2161	3964	464	-476	-4 5 0
ATOM	348	CA	LEU	44	5.117	32.592	55.959	1.000	26.76	
ANISOU	348	CA	LEU	44	4009	1973	4187	140	570	-9 8 6
ATOM	349	CB	LEU	44	5.978	31.585	56.727	1.000	28.25	
ANISOU	349	CB	LEU	44	5094	2194	3448	-153	277	-5 6 2
ATOM	350	CG	LEU	44	5.284	30.494	57.533	1.000	32.03	
ANISOU	350	CG	LEU	44	5971	2801	3398	-279	1192	-6 2 7
ATOM	351	CD1	LEU	44	4.485	29.535	56.656	1.000	37.95	
ANISOU	351	CD1	LEU	44	7665	2239	4514	-1148	2039	-1 4 0 3
ATOM	352	CD2	LEU	44	6.302	29.703	58.361	1.000	36.97	
ANISOU	352	CD2	LEU	44	7096	2869	4080	1150	2171	1 8 6
ATOM	353	C	LEU	44	4.000	33.145	56.841	1.000	31.10	
ANISOU	353	C	LEU	44	3835	3182	4800	-700	837	-2 2 0 5
ATOM	354	O	LEU	44	2.913	32.543	56.867	1.000	30.19	
ANISOU	354	O	LEU	44	4402	3299	3768	-1248	870	-2 1 6 5
ATOM	355	N	ALA	45	4.238	34.247	57.547	1.000	28.74	
ANISOU	355	N	ALA	45	2897	2938	5083	-562	710	-2 0 6 1
ATOM	356	CA	ALA	45	3.382	34.751	58.623	1.000	27.09	
ANISOU	356	CA	ALA	45	2716	2817	4761	-751	467	-2 1 4 0
ATOM	357	C	ALA	45	1.943	35.014	58.195	1.000	24.95	
ANISOU	357	C	ALA	45	2697	3110	3673	-784	709	-1 2 5 7
ATOM	358	O	ALA	45	1.021	34.515	58.875	1.000	22.50	
ANISOU	358	O	ALA	45	2762	2585	3201	-565	560	-1 1 4 6
ATOM	359	CB	ALA	45	3.975	36.005	59.248	1.000	36.30	
ANISOU	359	CB	ALA	45	3259	4219	6315	-1912	1332	-3 4 0 4
ATOM	360	N	SER	46	1.729	35.779	57.128	1.000	26.85	
ANISOU	360	N	SER	46	3258	3756	3187	-1732	618	-1 1 8 4
ATOM	361	CA	SER	46	0.380	36.052	56.642	1.000	24.97	
ANISOU	361	CA	SER	46	3686	3189	2611	-1223	511	-1 1 0 5
ATOM	362	CB	SER	46	0.422	36.950	55.392	1.000	32.35	
ANISOU	362	CB	SER	46	5428	3467	3395	-2232	70	-4 5 8
ATOM	363	OG	SER	46	0.630	38.289	55.772	1.000	45.77	
ANISOU	363	OG	SER	46	7730	3349	6313	-2746	2499	-8 0 7
ATOM	364	C	SER	46	-0.408	34.787	56.307	1.000	20.63	
ANISOU	364	C	SER	46	2797	2469	2572	-423	-151	-5 4 2
ATOM	365	O	SER	46	-1.578	34.672	56.698	1.000	21.93	
ANISOU	365	O	SER	46	3120	2486	2725	-559	305	-4 0 3
ATOM	366	N	ALA	47	0.211	33.855	55.590	1.000	22.39	
ANISOU	366	N	ALA	47	3096	2167	3244	-488	394	-3 6 8

- 102 -

ATOM	367	CA	ALA	47	-0.397	32.596	55.176	1.000	19.54	
ANISOU	367	CA	ALA	47	2746	1863	2814	-289	362	-18
ATOM	368	CB	ALA	47	0.548	31.900	54.191	1.000	23.54	
ANISOU	368	CB	ALA	47	3524	1717	3705	-617	1237	-159
ATOM	369	C	ALA	47	-0.715	31.714	56.381	1.000	19.95	
ANISOU	369	C	ALA	47	2282	2546	2752	-327	1925	7
ATOM	370	O	ALA	47	-1.836	31.199	56.518	1.000	19.66	
ANISOU	370	O	ALA	47	2489	2589	2393	-614	211	-165
ATOM	371	N	LYS	48	0.270	31.558	57.268	1.000	18.24	
ANISOU	371	N	LYS	48	2713	1966	2253	-210	-139	-912
ATOM	372	CA	LYS	48	0.042	30.782	58.486	1.000	19.33	
ANISOU	372	CA	LYS	48	2398	2625	2321	43	-312	-563
ATOM	373	C	LYS	48	-1.110	31.329	59.322	1.000	20.57	
ANISOU	373	C	LYS	48	2476	2556	2785	-326	83	-566
ATOM	374	O	LYS	48	-2.022	30.613	59.771	1.000	20.34	
ANISOU	374	O	LYS	48	3207	2598	1923	-521	139	-340
ATOM	375	CB	LYS	48	1.352	30.758	59.294	1.000	24.61	
ANISOU	375	CB	LYS	48	2400	3792	3158	-258	-556	-80
ATOM	376	CG	LYS	48	1.237	29.873	60.531	1.000	30.84	
ANISOU	376	CG	LYS	48	4306	4044	3366	-291	-1504	277
ATOM	377	CD	LYS	48	1.837	30.575	61.736	1.000	41.45	
ANISOU	377	CD	LYS	48	6742	5755	3251	-1067	-1382	-356
ATOM	378	CE	LYS	48	1.625	29.717	62.966	1.000	41.63	
ANISOU	378	CE	LYS	48	6620	6124	3073	-466	-1047	-353
ATOM	379	NZ	LYS	48	1.074	30.497	64.112	1.000	42.62	
ANISOU	379	NZ	LYS	48	5883	6866	3444	460	-1193	-425
ATOM	380	N	ASP	49	-1.110	32.625	59.607	1.000	19.18	
ANISOU	380	N	ASP	49	2348	2602	2337	-464	100	-806
ATOM	381	CA	ASP	49	-2.127	33.243	60.433	1.000	21.95	
ANISOU	381	CA	ASP	49	2555	2986	2801	-791	617	-1035
ATOM	382	CB	ASP	49	-1.868	34.756	60.611	1.000	23.97	
ANISOU	382	CB	ASP	49	2827	2872	3409	-250	-79	-1325
ATOM	383	CG	ASP	49	-0.681	35.078	61.492	1.000	25.41	
ANISOU	383	CG	ASP	49	2787	3405	3464	-365	113	-1866
ATOM	384	OD1	ASP	49	-0.153	34.153	62.143	1.000	30.75	
ANISOU	384	OD1	ASP	49	3572	4181	3932	-254	-967	-1667
ATOM	385	OD2	ASP	49	-0.235	36.256	61.563	1.000	30.78	
ANISOU	385	OD2	ASP	49	3303	3649	4742	-710	344	-2413
ATOM	386	C	ASP	49	-3.543	33.061	59.904	1.000	21.44	
ANISOU	386	C	ASP	49	2465	2651	3030	-388	540	-900
ATOM	387	O	ASP	49	-4.476	32.770	60.654	1.000	20.72	
ANISOU	387	O	ASP	49	2346	2181	3347	-279	550	-726
ATOM	388	N	LEU	50	-3.731	33.269	58.596	1.000	23.28	
ANISOU	388	N	LEU	50	2942	2712	3191	-1251	216	-644
ATOM	389	CA	LEU	50	-5.086	33.185	58.068	1.000	22.94	
ANISOU	389	CA	LEU	50	3104	1796	3815	-575	-205	-1079
ATOM	390	CB	LEU	50	-5.204	33.861	56.696	1.000	28.78	
ANISOU	390	CB	LEU	50	3948	2453	4535	-852	-755	-254
ATOM	391	CG	LEU	50	-6.620	34.246	56.260	1.000	25.30	
ANISOU	391	CG	LEU	50	3800	2294	3520	30	325	-531
ATOM	392	CD1	LEU	50	-7.552	34.478	57.441	1.000	44.77	
ANISOU	392	CD1	LEU	50	6382	4432	6196	-475	3026	-1060
ATOM	393	CD2	LEU	50	-6.625	35.485	55.385	1.000	32.52	
ANISOU	393	CD2	LEU	50	5861	1962	4533	752	354	-433
ATOM	394	C	LEU	50	-5.566	31.737	57.982	1.000	21.12	
ANISOU	394	C	LEU	50	2559	1870	3595	-643	742	-1270
ATOM	395	O	LEU	50	-6.772	31.494	58.175	1.000	21.13	
ANISOU	395	O	LEU	50	2491	2457	3083	-543	579	-1097
ATOM	396	N	VAL	51	-4.681	30.769	57.715	1.000	16.27	
ANISOU	396	N	VAL	51	2517	1843	1823	-302	-3	-646
ATOM	397	CA	VAL	51	-5.186	29.370	57.701	1.000	18.07	

- 103 -

ANISOU	397	CA	VAL	51	3154	1763	1947	-401	-15	-427
ATOM	398	CB	VAL	51	-4.281	28.415	56.889	1.000	16.07	
ANISOU	398	CB	VAL	51	2981	1629	1496	-621	-255	-501
ATOM	399	CG1	VAL	51	-3.002	28.114	57.668	1.000	18.99	
ANISOU	399	CG1	VAL	51	2959	2382	1875	-383	-100	302
ATOM	400	CG2	VAL	51	-5.006	27.119	56.497	1.000	22.16	
ANISOU	400	CG2	VAL	51	4569	2121	1728	-1393	64	-869
ATOM	401	C	VAL	51	-5.446	28.899	59.114	1.000	17.74	
ANISOU	401	C	VAL	51	2508	2223	2009	-435	142	-445
ATOM	402	O	VAL	51	-6.430	28.187	59.346	1.000	19.76	
ANISOU	402	O	VAL	51	3005	2160	2345	-692	726	-1021
ATOM	403	N	ILE	52	-4.671	29.263	60.125	1.000	20.23	
ANISOU	403	N	ILE	52	2980	2945	1760	-649	364	-902
ATOM	404	CA	ILE	52	-4.990	28.875	61.507	1.000	20.17	
ANISOU	404	CA	ILE	52	3200	2665	1800	-758	627	-1134
ATOM	405	CB	ILE	52	-3.847	29.230	62.469	1.000	21.31	
ANISOU	405	CB	ILE	52	3294	3151	1652	-449	462	-1043
ATOM	406	CG2	ILE	52	-4.238	29.178	63.931	1.000	21.29	
ANISOU	406	CG2	ILE	52	3543	2826	1719	-362	529	-689
ATOM	407	CG1	ILE	52	-2.619	28.346	62.217	1.000	25.37	
ANISOU	407	CG1	ILE	52	3213	3819	2608	-307	727	-1090
ATOM	408	CD1	ILE	52	-2.871	26.872	62.470	1.000	28.56	
ANISOU	408	CD1	ILE	52	3474	3578	3798	106	178	-1110
ATOM	409	C	ILE	52	-6.284	29.514	61.950	1.000	22.44	
ANISOU	409	C	ILE	52	3119	3216	2190	-710	645	-1228
ATOM	410	O	ILE	52	-7.072	28.856	62.647	1.000	23.23	
ANISOU	410	O	ILE	52	3390	3654	1781	-766	758	-1246
ATOM	411	N	ASP	53	-6.519	30.754	61.530	1.000	23.33	
ANISOU	411	N	ASP	53	2897	3064	2903	-626	700	-1361
ATOM	412	CA	ASP	53	-7.826	31.335	61.897	1.000	24.49	
ANISOU	412	CA	ASP	53	2818	3347	3141	-759	781	-1545
ATOM	413	CB	ASP	53	-7.942	32.781	61.411	1.000	27.43	
ANISOU	413	CB	ASP	53	2854	3335	4235	-434	819	-1446
ATOM	414	CG	ASP	53	-9.309	33.397	61.570	1.000	30.99	
ANISOU	414	CG	ASP	53	3166	4281	4326	36	1242	-1214
ATOM	415	OD1	ASP	53	-9.657	33.779	62.705	1.000	37.26	
ANISOU	415	OD1	ASP	53	4369	4569	5220	153	1263	-2733
ATOM	416	OD2	ASP	53	-10.050	33.491	60.553	1.000	38.45	
ANISOU	416	OD2	ASP	53	3393	6043	5173	810	557	-1648
ATOM	417	C	ASP	53	-8.953	30.495	61.316	1.000	24.64	
ANISOU	417	C	ASP	53	3028	3701	2634	-919	372	-1031
ATOM	418	O	ASP	53	-10.011	30.327	61.915	1.000	28.52	
ANISOU	418	O	ASP	53	3399	3835	3603	-1519	962	-2151
ATOM	419	N	PHE	54	-8.744	29.978	60.108	1.000	22.04	
ANISOU	419	N	PHE	54	2921	2974	2479	-573	174	-704
ATOM	420	CA	PHE	54	-9.772	29.187	59.432	1.000	19.99	
ANISOU	420	CA	PHE	54	2253	2879	2463	-421	771	-978
ATOM	421	CB	PHE	54	-9.423	29.030	57.942	1.000	18.45	
ANISOU	421	CB	PHE	54	2856	1983	2171	-65	426	-518
ATOM	422	CG	PHE	54	-10.493	28.292	57.145	1.000	21.36	
ANISOU	422	CG	PHE	54	3063	2735	2318	-646	599	-627
ATOM	423	CD1	PHE	54	-11.714	28.906	56.933	1.000	23.18	
ANISOU	423	CD1	PHE	54	3199	2783	2826	-703	-29	-624
ATOM	424	CD2	PHE	54	-10.293	27.035	56.619	1.000	23.32	
ANISOU	424	CD2	PHE	54	3482	2802	2577	-689	212	-858
ATOM	425	CE1	PHE	54	-12.719	28.291	56.241	1.000	26.45	
ANISOU	425	CE1	PHE	54	3345	3696	3008	-1418	129	-554
ATOM	426	CE2	PHE	54	-11.303	26.375	55.921	1.000	25.65	
ANISOU	426	CE2	PHE	54	3750	3815	2182	-1404	607	-1005
ATOM	427	CZ	PHE	54	-12.522	27.013	55.725	1.000	26.17	
ANISOU	427	CZ	PHE	54	3433	3830	2679	-1829	298	-813

- 104 -

ATOM	428	C	PHE	54	-9.959	27.854	60.132	1.000	19.44	
ANISOU	428	C	PHE	54	2340	3430	1617	-834	319	-759
ATOM	429	O	PHE	54	-11.087	27.450	60.386	1.000	22.11	
ANISOU	429	O	PHE	54	2601	3066	2734	-948	1018	-1466
ATOM	430	N	PHE	55	-8.882	27.166	60.448	1.000	20.59	
ANISOU	430	N	PHE	55	2728	3375	1720	-666	180	-611
ATOM	431	CA	PHE	55	-8.966	25.927	61.212	1.000	22.59	
ANISOU	431	CA	PHE	55	3092	3671	1820	-728	381	-372
ATOM	432	CB	PHE	55	-7.579	25.360	61.478	1.000	21.93	
ANISOU	432	CB	PHE	55	3163	3622	1549	-692	287	-158
ATOM	433	CG	PHE	55	-6.790	24.833	60.284	1.000	20.60	
ANISOU	433	CG	PHE	55	3034	2998	1793	-1004	365	-375
ATOM	434	CD1	PHE	55	-7.352	24.526	59.057	1.000	18.72	
ANISOU	434	CD1	PHE	55	2300	3095	1717	-1078	586	-271
ATOM	435	CD2	PHE	55	-5.430	24.615	60.385	1.000	18.06	
ANISOU	435	CD2	PHE	55	3132	2490	1241	-926	128	-497
ATOM	436	CE1	PHE	55	-6.609	24.037	58.014	1.000	18.92	
ANISOU	436	CE1	PHE	55	2455	2761	1971	-844	436	-542
ATOM	437	CE2	PHE	55	-4.672	24.124	59.352	1.000	18.58	
ANISOU	437	CE2	PHE	55	3291	2606	1163	-478	63	-299
ATOM	438	CZ	PHE	55	-5.256	23.814	58.134	1.000	17.68	
ANISOU	438	CZ	PHE	55	2660	2567	1490	-380	129	-806
ATOM	439	C	PHE	55	-9.684	26.111	62.546	1.000	24.99	
ANISOU	439	C	PHE	55	3310	4138	2046	-830	647	-415
ATOM	440	O	PHE	55	-10.532	25.281	62.872	1.000	30.29	
ANISOU	440	O	PHE	55	3802	4943	2763	-1527	1314	-1102
ATOM	441	N	GLU	56	-9.330	27.144	63.311	1.000	23.65	
ANISOU	441	N	GLU	56	2864	4109	2013	-634	937	-525
ATOM	442	CA	GLU	56	-9.868	27.355	64.636	1.000	30.01	
ANISOU	442	CA	GLU	56	3632	5378	2394	-1050	1465	-994
ATOM	443	CB	GLU	56	-8.998	28.333	65.436	1.000	36.40	
ANISOU	443	CB	GLU	56	4531	6933	2367	-1606	1318	-1623
ATOM	444	CG	GLU	56	-7.666	27.827	65.916	1.000	41.89	
ANISOU	444	CG	GLU	56	5006	8196	2713	-1457	404	-1900
ATOM	445	CD	GLU	56	-6.787	28.880	66.575	1.000	48.94	
ANISOU	445	CD	GLU	56	6081	9310	3202	-2278	-73	-2062
ATOM	446	OE1	GLU	56	-5.694	28.515	67.078	1.000	60.73	
ANISOU	446	OE1	GLU	56	8034	12274	2769	-3208	-2335	266
ATOM	447	OE2	GLU	56	-7.145	30.084	66.614	1.000	58.51	
ANISOU	447	OE2	GLU	56	8742	9338	4151	-2088	1096	-3951
ATOM	448	C	GLU	56	-11.289	27.920	64.617	1.000	30.60	
ANISOU	448	C	GLU	56	3764	4923	2941	-977	1967	-1271
ATOM	449	O	GLU	56	-12.058	27.542	65.504	1.000	35.21	
ANISOU	449	O	GLU	56	4384	5304	3690	-1136	2652	-1235
ATOM	450	N	HIS	57	-11.603	28.805	63.673	1.000	30.00	
ANISOU	450	N	HIS	57	3730	4846	2823	-654	1684	-1582
ATOM	451	CA	HIS	57	-12.854	29.559	63.759	1.000	33.51	
ANISOU	451	CA	HIS	57	3853	5101	3778	-519	1673	-1911
ATOM	452	CB	HIS	57	-12.536	31.046	63.991	1.000	33.40	
ANISOU	452	CB	HIS	57	3844	5183	3664	-411	1546	-2250
ATOM	453	CG	HIS	57	-11.577	31.344	65.095	1.000	35.13	
ANISOU	453	CG	HIS	57	4497	5409	3444	-505	1340	-1992
ATOM	454	CD2	HIS	57	-10.361	31.946	65.071	1.000	35.26	
ANISOU	454	CD2	HIS	57	4837	5214	3345	-834	637	-1456
ATOM	455	ND1	HIS	57	-11.819	31.021	66.411	1.000	40.52	
ANISOU	455	ND1	HIS	57	6021	5885	3490	-1360	1474	-2002
ATOM	456	CE1	HIS	57	-10.798	31.410	67.151	1.000	42.28	
ANISOU	456	CE1	HIS	57	6680	6066	3320	-1632	1099	-1772
ATOM	457	NE2	HIS	57	-9.902	31.970	66.362	1.000	41.69	
ANISOU	457	NE2	HIS	57	6377	6133	3329	-1817	407	-1148
ATOM	458	C	HIS	57	-13.769	29.466	62.547	1.000	32.58	

ANISOU	458	C	HIS	57	3083	5097	4199	-729	1723	-2066
ATOM	459	O	HIS	57	-14.902	29.965	62.578	1.000	33.80	
ANISOU	459	O	HIS	57	3121	5097	4625	-731	1865	-2565
ATOM	460	N	GLY	58	-13.370	28.866	61.432	1.000	28.78	
ANISOU	460	N	GLY	58	2841	4353	3742	-253	1341	-1506
ATOM	461	CA	GLY	58	-14.326	28.685	60.332	1.000	26.99	
ANISOU	461	CA	GLY	58	2471	3916	3869	24	1298	-1173
ATOM	462	C	GLY	58	-15.447	27.737	60.738	1.000	29.94	
ANISOU	462	C	GLY	58	2665	4357	4353	-261	1323	-1058
ATOM	463	O	GLY	58	-15.241	26.805	61.534	1.000	29.23	
ANISOU	463	O	GLY	58	2976	4044	4087	-571	1192	-1297
ATOM	464	N	SER	59	-16.635	27.958	60.193	1.000	27.61	
ANISOU	464	N	SER	59	2556	3905	4029	-108	1461	-1767
ATOM	465	CA	SER	59	-17.812	27.153	60.497	1.000	28.42	
ANISOU	465	CA	SER	59	2675	4074	4049	-189	1294	-1325
ATOM	466	CB	SER	59	-19.121	27.889	60.162	1.000	28.29	
ANISOU	466	CB	SER	59	2556	4574	3618	-339	1198	-928
ATOM	467	OG	SER	59	-19.229	27.978	58.739	1.000	28.66	
ANISOU	467	OG	SER	59	3598	3742	3547	166	1729	-867
ATOM	468	C	SER	59	-17.795	25.843	59.724	1.000	29.57	
ANISOU	468	C	SER	59	3467	3990	3779	-646	1463	-1206
ATOM	469	O	SER	59	-16.990	25.651	58.810	1.000	22.72	
ANISOU	469	O	SER	59	3054	3042	2537	-144	648	-369
ATOM	470	N	GLU	60	-18.698	24.939	60.103	1.000	26.90	
ANISOU	470	N	GLU	60	2413	3900	3907	-69	1079	-853
ATOM	471	CA	GLU	60	-18.699	23.684	59.359	1.000	26.98	
ANISOU	471	CA	GLU	60	2699	3515	4037	-98	709	-537
ATOM	472	CB	GLU	60	-19.646	22.681	60.001	1.000	39.11	
ANISOU	472	CB	GLU	60	5393	4393	5075	-1361	908	364
ATOM	473	CG	GLU	60	-19.011	21.665	60.917	1.000	44.63	
ANISOU	473	CG	GLU	60	5606	5473	5878	-977	1079	1219
ATOM	474	CD	GLU	60	-17.507	21.543	60.797	1.000	48.52	
ANISOU	474	CD	GLU	60	5714	6217	6503	-390	1207	877
ATOM	475	OE1	GLU	60	-17.030	21.223	59.684	1.000	48.11	
ANISOU	475	OE1	GLU	60	5349	7545	5384	709	366	1951
ATOM	476	OE2	GLU	60	-16.828	21.763	61.829	1.000	46.50	
ANISOU	476	OE2	GLU	60	4926	5742	7000	1158	1550	-1504
ATOM	477	C	GLU	60	-19.091	23.960	57.915	1.000	25.30	
ANISOU	477	C	GLU	60	2829	2728	4055	86	725	-656
ATOM	478	O	GLU	60	-18.529	23.346	57.027	1.000	24.18	
ANISOU	478	O	GLU	60	2119	2980	4091	-202	741	-752
ATOM	479	N	ALA	61	-20.032	24.890	57.716	1.000	25.58	
ANISOU	479	N	ALA	61	2083	3206	4432	-34	612	-774
ATOM	480	CA	ALA	61	-20.495	25.212	56.368	1.000	24.05	
ANISOU	480	CA	ALA	61	1838	2999	4301	228	720	-1055
ATOM	481	CB	ALA	61	-21.670	26.176	56.459	1.000	27.53	
ANISOU	481	CB	ALA	61	2807	1857	5797	394	704	-606
ATOM	482	C	ALA	61	-19.385	25.790	55.500	1.000	27.31	
ANISOU	482	C	ALA	61	3170	2572	4633	-377	1178	-1026
ATOM	483	O	ALA	61	-19.247	25.467	54.311	1.000	22.29	
ANISOU	483	O	ALA	61	2363	1876	4232	42	661	-319
ATOM	484	N	GLU	62	-18.580	26.642	56.118	1.000	22.18	
ANISOU	484	N	GLU	62	2075	2258	4094	396	569	-394
ATOM	485	CA	GLU	62	-17.455	27.258	55.416	1.000	24.19	
ANISOU	485	CA	GLU	62	2401	2603	4188	150	852	-590
ATOM	486	CB	GLU	62	-16.806	28.354	56.277	1.000	24.68	
ANISOU	486	CB	GLU	62	2401	2490	4485	91	1273	-828
ATOM	487	CG	GLU	62	-17.641	29.636	56.356	1.000	25.19	
ANISOU	487	CG	GLU	62	2542	2620	4409	353	421	-685
ATOM	488	CD	GLU	62	-17.288	30.581	57.480	1.000	29.27	
ANISOU	488	CD	GLU	62	3284	2991	4845	621	515	-1290

- 106 -

ATOM	489	OE1	GLU	62	-16.527	30.241	58.410	1.000	30.11	
ANISOU	489	OE1	GLU	62	3231	3067	5143	318	56	-1639
ATOM	490	OE2	GLU	62	-17.796	31.739	57.436	1.000	35.30	
ANISOU	490	OE2	GLU	62	4832	2994	5584	863	109	-1327
ATOM	491	C	GLU	62	-16.409	26.226	55.025	1.000	21.70	
ANISOU	491	C	GLU	62	2394	2421	3430	30	784	-579
ATOM	492	O	GLU	62	-15.818	26.218	53.940	1.000	19.44	
ANISOU	492	O	GLU	62	2095	2140	3153	-301	467	-604
ATOM	493	N	LYS	63	-16.184	25.308	55.972	1.000	20.08	
ANISOU	493	N	LYS	63	2472	2266	2893	-74	761	-902
ATOM	494	CA	LYS	63	-15.246	24.227	55.678	1.000	19.73	
ANISOU	494	CA	LYS	63	2322	2559	2614	133	429	-903
ATOM	495	CB	LYS	63	-14.934	23.497	56.988	1.000	18.48	
ANISOU	495	CB	LYS	63	1803	2743	2476	-218	587	-836
ATOM	496	CG	LYS	63	-13.946	24.240	57.881	1.000	19.17	
ANISOU	496	CG	LYS	63	2115	2332	2836	-296	325	-674
ATOM	497	CD	LYS	63	-13.839	23.651	59.290	1.000	26.23	
ANISOU	497	CD	LYS	63	2978	4084	2902	-888	-177	-287
ATOM	498	CE	LYS	63	-12.753	24.383	60.068	1.000	27.75	
ANISOU	498	CE	LYS	63	3074	5008	2461	-1239	500	-1082
ATOM	499	NZ	LYS	63	-12.929	24.378	61.530	1.000	34.95	
ANISOU	499	NZ	LYS	63	3177	7579	2524	-2594	840	-894
ATOM	500	C	LYS	63	-15.789	23.304	54.586	1.000	17.52	
ANISOU	500	C	LYS	63	2014	2191	2453	51	529	-691
ATOM	501	O	LYS	63	-15.025	22.953	53.654	1.000	17.58	
ANISOU	501	O	LYS	63	2266	1709	2704	158	707	-653
ATOM	502	N	ARG	64	-17.069	22.912	54.641	1.000	19.63	
ANISOU	502	N	ARG	64	2081	2452	2926	-14	614	-592
ATOM	503	CA	ARG	64	-17.618	22.041	53.595	1.000	19.00	
ANISOU	503	CA	ARG	64	1509	2526	3185	-3	620	-652
ATOM	504	C	ARG	64	-17.471	22.634	52.194	1.000	20.42	
ANISOU	504	C	ARG	64	2165	2436	3157	-390	-22	-536
ATOM	505	O	ARG	64	-17.204	21.934	51.195	1.000	18.83	
ANISOU	505	O	ARG	64	1854	2184	3115	-434	575	-201
ATOM	506	CB	ARG	64	-19.080	21.670	53.871	1.000	24.70	
ANISOU	506	CB	ARG	64	1470	3652	4263	-51	841	-909
ATOM	507	CG	ARG	64	-19.838	20.933	52.795	1.000	36.49	
ANISOU	507	CG	ARG	64	2961	5284	5621	-2020	138	-882
ATOM	508	CD	ARG	64	-21.315	20.645	53.095	1.000	46.32	
ANISOU	508	CD	ARG	64	3034	6962	7603	-2438	327	-1187
ATOM	509	NE	ARG	64	-21.776	21.216	54.331	1.000	55.81	
ANISOU	509	NE	ARG	64	3917	8636	8652	-3960	2222	-1870
ATOM	510	CZ	ARG	64	-22.814	21.840	54.811	1.000	58.82	
ANISOU	510	CZ	ARG	64	4438	8939	8972	-3479	1988	-2480
ATOM	511	NH1	ARG	64	-23.884	22.106	54.071	1.000	76.83	
ANISOU	511	NH1	ARG	64	6024	9527	13641	-1787	-165	-1872
ATOM	512	NH2	ARG	64	-22.797	22.213	56.093	1.000	69.53	
ANISOU	512	NH2	ARG	64	7792	9201	9424	-5884	3891	-3304
ATOM	513	N	ALA	65	-17.621	23.947	52.066	1.000	20.43	
ANISOU	513	N	ALA	65	1689	2554	3519	24	612	-525
ATOM	514	CA	ALA	65	-17.505	24.656	50.782	1.000	19.45	
ANISOU	514	CA	ALA	65	1649	2216	3523	409	184	-553
ATOM	515	CB	ALA	65	-17.912	26.108	50.984	1.000	23.73	
ANISOU	515	CB	ALA	65	1420	2019	5579	126	-373	-742
ATOM	516	C	ALA	65	-16.118	24.549	50.168	1.000	17.89	
ANISOU	516	C	ALA	65	1524	2099	3173	-47	108	-101
ATOM	517	O	ALA	65	-15.983	24.732	48.954	1.000	18.77	
ANISOU	517	O	ALA	65	1830	2178	3123	122	-8	-229
ATOM	518	N	VAL	66	-15.100	24.248	50.973	1.000	17.99	
ANISOU	518	N	VAL	66	1547	2151	3137	-86	36	-196
ATOM	519	CA	VAL	66	-13.746	24.066	50.430	1.000	16.74	

- 107 -

ANISOU 519	CA	VAL	66	1553	1959	2948	-62	-56	-2 5 4
ATOM 520	CB	VAL	66	-12.775	25.151	50.951	1.000	17.29	
ANISOU 520	CB	VAL	66	1805	1804	2963	-330	338	-1 8 5
ATOM 521	CG1	VAL	66	-13.238	26.532	50.455	1.000	16.70	
ANISOU 521	CG1	VAL	66	1547	1800	2997	111	545	-5 5 3
ATOM 522	CG2	VAL	66	-12.652	25.180	52.462	1.000	18.65	
ANISOU 522	CG2	VAL	66	2053	1996	3036	-193	17	-5 3 8
ATOM 523	C	VAL	66	-13.201	22.680	50.724	1.000	15.66	
ANISOU 523	C	VAL	66	1775	1813	2362	-70	-250	-4 5 7
ATOM 524	O	VAL	66	-11.972	22.493	50.808	1.000	14.19	
ANISOU 524	O	VAL	66	1747	1576	2069	-122	-56	-3 4 7
ATOM 525	N	THR	67	-14.071	21.695	50.873	1.000	14.46	
ANISOU 525	N	THR	67	1550	1602	2343	126	-48	-7 2 2
ATOM 526	CA	THR	67	-13.723	20.279	51.000	1.000	14.06	
ANISOU 526	CA	THR	67	1461	1698	2185	234	5	-7 4 0
ATOM 527	CB	THR	67	-14.419	19.647	52.225	1.000	15.08	
ANISOU 527	CB	THR	67	1721	1955	2053	-51	-426	-4 4 4
ATOM 528	OG1	THR	67	-14.089	20.337	53.453	1.000	17.41	
ANISOU 528	OG1	THR	67	2538	1949	2128	-39	70	-7 1 6
ATOM 529	CG2	THR	67	-13.915	18.215	52.420	1.000	16.63	
ANISOU 529	CG2	THR	67	2182	1888	2248	148	293	-6 5 8
ATOM 530	C	THR	67	-14.067	19.518	49.728	1.000	12.37	
ANISOU 530	C	THR	67	1144	1422	2132	209	-95	-5 1 7
ATOM 531	O	THR	67	-15.208	19.567	49.229	1.000	14.82	
ANISOU 531	O	THR	67	1197	2086	2350	208	-168	-3 6 2
ATOM 532	N	SER	68	-13.092	18.790	49.180	1.000	11.61	
ANISOU 532	N	SER	68	1109	1421	1881	37	-58	-5 3 4
ATOM 533	CA	SER	68	-13.306	17.955	48.003	1.000	11.45	
ANISOU 533	CA	SER	68	1274	1444	1631	-49	-30	-3 7 4
ATOM 534	CB	SER	68	-12.027	17.317	47.480	1.000	11.88	
ANISOU 534	CB	SER	68	1446	1523	1544	79	252	-1 5 7
ATOM 535	OG	SER	68	-11.026	18.292	47.239	1.000	16.95	
ANISOU 535	OG	SER	68	1557	2314	2569	-336	389	-2 1 8
ATOM 536	C	SER	68	-14.269	16.815	48.319	1.000	11.56	
ANISOU 536	C	SER	68	1287	1375	1732	-61	53	-4 0 6
ATOM 537	O	SER	68	-14.308	16.384	49.476	1.000	14.62	
ANISOU 537	O	SER	68	1998	1860	1697	-538	153	-4 3 0
ATOM 538	N	PRO	69	-15.026	16.324	47.344	1.000	12.78	
ANISOU 538	N	PRO	69	1476	1473	1905	-243	-88	-1 9 4
ATOM 539	CD	PRO	69	-15.130	16.801	45.953	1.000	12.47	
ANISOU 539	CD	PRO	69	1022	1808	1909	-199	-203	-1 4 4
ATOM 540	CA	PRO	69	-15.941	15.214	47.639	1.000	12.21	
ANISOU 540	CA	PRO	69	1358	1369	1913	-178	148	-4 3 7
ATOM 541	CB	PRO	69	-16.825	15.193	46.355	1.000	13.94	
ANISOU 541	CB	PRO	69	1362	1591	2343	-251	-178	-1 4
ATOM 542	CG	PRO	69	-15.924	15.715	45.290	1.000	14.38	
ANISOU 542	CG	PRO	69	1396	1947	2122	-554	-511	1 7 8
ATOM 543	C	PRO	69	-15.270	13.882	47.912	1.000	13.25	
ANISOU 543	C	PRO	69	1206	1526	2303	-217	-115	-1 0 0
ATOM 544	O	PRO	69	-15.932	12.985	48.481	1.000	14.01	
ANISOU 544	O	PRO	69	1753	1450	2122	-373	99	-3 0 1
ATOM 545	N	VAL	70	-14.015	13.692	47.554	1.000	13.46	
ANISOU 545	N	VAL	70	1288	1479	2348	-174	-108	-2 6 5
ATOM 546	CA	VAL	70	-13.184	12.548	47.898	1.000	13.49	
ANISOU 546	CA	VAL	70	1404	1692	2030	37	138	-1 9 5
ATOM 547	CB	VAL	70	-12.587	11.720	46.737	1.000	16.39	
ANISOU 547	CB	VAL	70	2142	1648	2439	-225	614	-4 5 2
ATOM 548	CG1	VAL	70	-13.615	10.756	46.208	1.000	33.50	
ANISOU 548	CG1	VAL	70	6470	2984	3274	-2702	41	-8 6 7
ATOM 549	CG2	VAL	70	-11.995	12.613	45.640	1.000	16.46	
ANISOU 549	CG2	VAL	70	1749	2234	2273	269	444	2 3

- 108 -

ATOM	550	C	VAL	70	-12.042	13.057	48.782	1.000	13.59	
ANISOU	550	C	VAL	70	1618	1382	2163	-38	-114	1 2 7
ATOM	551	O	VAL	70	-11.426	14.105	48.493	1.000	14.20	
ANISOU	551	O	VAL	70	1748	1685	1964	-265	26	1 8 2
ATOM	552	N	PRO	71	-11.786	12.365	49.898	1.000	14.21	
ANISOU	552	N	PRO	71	1607	1507	2285	-115	-62	3 1 0
ATOM	553	CD	PRO	71	-12.432	11.125	50.378	1.000	14.70	
ANISOU	553	CD	PRO	71	1920	1590	2076	-201	646	4
ATOM	554	CA	PRO	71	-10.830	12.919	50.878	1.000	17.41	
ANISOU	554	CA	PRO	71	2429	2008	2178	-522	-342	4 1 8
ATOM	555	CB	PRO	71	-11.338	12.304	52.193	1.000	20.87	
ANISOU	555	CB	PRO	71	3768	2082	2081	-743	190	1 4
ATOM	556	CG	PRO	71	-11.908	10.989	51.775	1.000	18.28	
ANISOU	556	CG	PRO	71	3534	1665	1746	-338	781	- 5 4
ATOM	557	C	PRO	71	-9.384	12.543	50.619	1.000	17.14	
ANISOU	557	C	PRO	71	2183	2304	2026	-684	-815	4 4
ATOM	558	O	PRO	71	-8.730	11.796	51.330	1.000	20.54	
ANISOU	558	O	PRO	71	2745	2610	2448	-87	-404	4 1 4
ATOM	559	N	THR	72	-8.834	13.111	49.556	1.000	16.59	
ANISOU	559	N	THR	72	2156	2046	2103	-235	-508	- 1 7
ATOM	560	CA	THR	72	-7.496	12.818	49.090	1.000	17.43	
ANISOU	560	CA	THR	72	2113	1884	2626	-254	-510	- 2 8 8
ATOM	561	CB	THR	72	-7.477	12.829	47.545	1.000	15.98	
ANISOU	561	CB	THR	72	1700	1761	2611	211	-458	- 4 2 1
ATOM	562	OG1	THR	72	-8.027	14.094	47.128	1.000	17.28	
ANISOU	562	OG1	THR	72	2146	1553	2868	27	-355	- 2 7 1
ATOM	563	CG2	THR	72	-8.348	11.764	46.929	1.000	12.63	
ANISOU	563	CG2	THR	72	1296	1581	1923	-46	328	- 1 2 7
ATOM	564	C	THR	72	-6.418	13.805	49.549	1.000	17.83	
ANISOU	564	C	THR	72	2153	1773	2847	-155	-1228	2 3 2
ATOM	565	O	THR	72	-5.216	13.536	49.329	1.000	20.17	
ANISOU	565	O	THR	72	2142	2265	3257	-225	-1049	4 8 0
ATOM	566	N	MET	73	-6.785	14.920	50.169	1.000	19.43	
ANISOU	566	N	MET	73	2876	2052	2455	-782	-451	- 1 4 4
ATOM	567	CA	MET	73	-5.799	15.944	50.521	1.000	18.75	
ANISOU	567	CA	MET	73	2117	2326	2682	-538	-466	- 2 8 0
ATOM	568	CB	MET	73	-4.758	15.338	51.480	1.000	22.03	
ANISOU	568	CB	MET	73	1826	2825	3718	-377	-306	5 9 5
ATOM	569	CG	MET	73	-5.374	15.059	52.843	1.000	27.01	
ANISOU	569	CG	MET	73	3545	2853	3864	-84	-87	1 5 2 6
ATOM	570	SD	MET	73	-4.107	14.850	54.107	1.000	32.23	
ANISOU	570	SD	MET	73	4364	4245	3637	469	-400	5 8 3
ATOM	571	CE	MET	73	-3.179	13.492	53.374	1.000	26.74	
ANISOU	571	CE	MET	73	2885	4895	2381	326	425	1 3 4 8
ATOM	572	C	MET	73	-5.066	16.582	49.355	1.000	17.20	
ANISOU	572	C	MET	73	1338	2129	3067	-20	-269	- 1 7 5
ATOM	573	O	MET	73	-3.945	17.110	49.498	1.000	21.20	
ANISOU	573	O	MET	73	1713	2512	3832	-541	51	- 1 0 2 4
ATOM	574	N	ARG	74	-5.630	16.600	48.175	1.000	18.64	
ANISOU	574	N	ARG	74	1881	2051	3150	84	-461	5 4 3
ATOM	575	CA	ARG	74	-5.091	17.180	46.967	1.000	15.73	
ANISOU	575	CA	ARG	74	937	1986	3053	169	27	- 1 7 4
ATOM	576	CB	ARG	74	-5.655	16.537	45.704	1.000	16.53	
ANISOU	576	CB	ARG	74	1711	1434	3137	-263	142	- 1 6 0
ATOM	577	CG	ARG	74	-4.911	16.934	44.440	1.000	15.01	
ANISOU	577	CG	ARG	74	1270	1288	3144	-156	279	- 5 5 4
ATOM	578	CD	ARG	74	-5.683	16.543	43.185	1.000	16.10	
ANISOU	578	CD	ARG	74	1967	1031	3120	268	-92	- 4 0 7
ATOM	579	NE	ARG	74	-4.902	16.816	41.966	1.000	18.81	
ANISOU	579	NE	ARG	74	2259	1813	3075	-432	-252	- 2 9 6
ATOM	580	CZ	ARG	74	-5.033	17.824	41.130	1.000	16.64	

- 109 -

ANISOU	580	CZ	ARG	74	1968	1646	2709	-141	-190	-596
ATOM	581	NH1	ARG	74	-5.951	18.775	41.293	1.000	20.09	
ANISOU	581	NH1	ARG	74	1899	2075	3660	54	-353	-788
ATOM	582	NH2	ARG	74	-4.220	17.896	40.068	1.000	20.12	
ANISOU	582	NH2	ARG	74	2366	2844	2437	153	-196	-400
ATOM	583	C	ARG	74	-5.373	18.681	46.966	1.000	12.70	
ANISOU	583	C	ARG	74	1187	1880	1758	6	-22	-136
ATOM	584	O	ARG	74	-4.501	19.465	46.582	1.000	14.07	
ANISOU	584	O	ARG	74	1049	2048	2247	-221	-170	-480
ATOM	585	N	ARG	75	-6.567	19.099	47.387	1.000	12.72	
ANISOU	585	N	ARG	75	1402	1702	1728	95	182	-108
ATOM	586	CA	ARG	75	-7.006	20.471	47.308	1.000	13.40	
ANISOU	586	CA	ARG	75	1924	1618	1548	87	275	-193
ATOM	587	CB	ARG	75	-7.737	20.784	45.995	1.000	13.45	
ANISOU	587	CB	ARG	75	1972	1387	1751	-179	51	-9
ATOM	588	CG	ARG	75	-6.908	20.637	44.721	1.000	13.38	
ANISOU	588	CG	ARG	75	1638	1851	1594	78	-217	101
ATOM	589	CD	ARG	75	-5.849	21.708	44.582	1.000	12.85	
ANISOU	589	CD	ARG	75	1537	1602	1741	237	62	-15
ATOM	590	NE	ARG	75	-5.087	21.685	43.347	1.000	13.71	
ANISOU	590	NE	ARG	75	1708	1797	1705	188	90	-91
ATOM	591	CZ	ARG	75	-3.984	21.036	43.013	1.000	12.46	
ANISOU	591	CZ	ARG	75	1348	1656	1731	-89	86	117
ATOM	592	NH1	ARG	75	-3.418	20.241	43.894	1.000	14.64	
ANISOU	592	NH1	ARG	75	1933	1794	1834	186	-91	65
ATOM	593	NH2	ARG	75	-3.444	21.167	41.794	1.000	13.72	
ANISOU	593	NH2	ARG	75	1510	2037	1667	-136	84	-83
ATOM	594	C	ARG	75	-7.948	20.787	48.475	1.000	12.74	
ANISOU	594	C	ARG	75	1400	1656	1784	-209	214	-464
ATOM	595	O	ARG	75	-8.780	19.944	48.818	1.000	14.60	
ANISOU	595	O	ARG	75	1348	1926	2273	-427	156	-480
ATOM	596	N	GLY	76	-7.830	21.955	49.078	1.000	11.92	
ANISOU	596	N	GLY	76	1268	1537	1724	-22	34	-389
ATOM	597	CA	GLY	76	-8.801	22.395	50.070	1.000	12.44	
ANISOU	597	CA	GLY	76	1439	1493	1796	-315	263	-412
ATOM	598	C	GLY	76	-8.536	21.857	51.469	1.000	12.50	
ANISOU	598	C	GLY	76	1324	1527	1900	5	326	-273
ATOM	599	O	GLY	76	-7.388	21.517	51.769	1.000	14.25	
ANISOU	599	O	GLY	76	1100	2099	2218	-277	239	-225
ATOM	600	N	PHE	77	-9.574	21.840	52.287	1.000	12.65	
ANISOU	600	N	PHE	77	1191	1806	1809	-162	231	-351
ATOM	601	CA	PHE	77	-9.526	21.474	53.694	1.000	14.00	
ANISOU	601	CA	PHE	77	1295	2110	1914	-260	276	-138
ATOM	602	CB	PHE	77	-10.644	22.226	54.451	1.000	14.73	
ANISOU	602	CB	PHE	77	1554	2169	1874	-402	485	-317
ATOM	603	CG	PHE	77	-10.773	21.824	55.912	1.000	17.13	
ANISOU	603	CG	PHE	77	1927	2730	1849	-374	378	-243
ATOM	604	CD1	PHE	77	-9.949	22.369	56.886	1.000	19.49	
ANISOU	604	CD1	PHE	77	2744	2700	1962	-119	219	-789
ATOM	605	CD2	PHE	77	-11.730	20.902	56.309	1.000	19.13	
ANISOU	605	CD2	PHE	77	2348	3068	1852	-501	864	-165
ATOM	606	CE1	PHE	77	-10.068	21.973	58.217	1.000	19.75	
ANISOU	606	CE1	PHE	77	2956	2381	2168	-174	-313	-304
ATOM	607	CE2	PHE	77	-11.829	20.479	57.627	1.000	18.73	
ANISOU	607	CE2	PHE	77	2565	2711	1841	-382	310	-77
ATOM	608	CZ	PHE	77	-10.986	21.013	58.584	1.000	19.22	
ANISOU	608	CZ	PHE	77	2378	2542	2382	98	13	-364
ATOM	609	C	PHE	77	-9.668	19.976	53.924	1.000	13.73	
ANISOU	609	C	PHE	77	1306	2096	1813	-368	21	-204
ATOM	610	O	PHE	77	-10.520	19.313	53.291	1.000	16.02	
ANISOU	610	O	PHE	77	1386	2508	2194	-470	-128	-425

- 110 -

ATOM 611 N THR 78 -8.869 19.439 54.852 1.000 14.33
 ANISOU 611 N THR 78 1543 2270 1629 -472 35 -49
 ATOM 612 CA THR 78 -9.034 18.053 55.276 1.000 15.80
 ANISOU 612 CA THR 78 1813 2310 1880 -508 -23 8 2
 ATOM 613 CB THR 78 -8.001 17.081 54.666 1.000 18.26
 ANISOU 613 CB THR 78 1583 2199 3158 -599 334 1 3 1
 ATOM 614 OG1 THR 78 -7.924 17.323 53.266 1.000 21.81
 ANISOU 614 OG1 THR 78 3351 1877 3057 -88 943 -370
 ATOM 615 CG2 THR 78 -8.419 15.634 54.888 1.000 20.35
 ANISOU 615 CG2 THR 78 2855 2254 2622 -1119 1108 -707
 ATOM 616 C THR 78 -8.832 17.881 56.777 1.000 19.14
 ANISOU 616 C THR 78 2845 2479 1948 -1747 -471 1 6 9
 ATOM 617 O THR 78 -7.801 18.311 57.290 1.000 22.04
 ANISOU 617 O THR 78 2781 2889 2704 -1718 -985 7 6 3
 ATOM 618 N GLY 79 -9.730 17.203 57.484 1.000 19.20
 ANISOU 618 N GLY 79 2629 2823 1844 -1352 19 4 5
 ATOM 619 CA GLY 79 -9.429 16.695 58.819 1.000 16.69
 ANISOU 619 CA GLY 79 1800 2770 1771 -518 196 -9 5
 ATOM 620 C GLY 79 -8.672 15.376 58.720 1.000 22.98
 ANISOU 620 C GLY 79 2381 2874 3477 -272 -289 -5 4 5
 ATOM 621 O GLY 79 -9.227 14.504 58.044 1.000 25.57
 ANISOU 621 O GLY 79 3683 2520 3514 -456 -974 -1 4 1
 ATOM 622 N LEU 80 -7.494 15.236 59.319 1.000 22.91
 ANISOU 622 N LEU 80 2412 2900 3392 30 -206 -6 0 6
 ATOM 623 CA LEU 80 -6.644 14.081 59.072 1.000 25.08
 ANISOU 623 CA LEU 80 2848 2777 3904 206 621 3 6 1
 ATOM 624 C LEU 80 -6.372 13.294 60.370 1.000 24.30
 ANISOU 624 C LEU 80 2834 2762 3637 -300 480 2 0 0
 ATOM 625 O LEU 80 -5.729 13.812 61.291 1.000 25.14
 ANISOU 625 O LEU 80 2253 3017 4283 27 145 -5
 ATOM 626 CB LEU 80 -5.318 14.480 58.415 1.000 27.16
 ANISOU 626 CB LEU 80 3057 3326 3937 379 918 6 4 1
 ATOM 627 CG LEU 80 -4.411 13.338 57.933 1.000 29.43
 ANISOU 627 CG LEU 80 3474 3505 4204 287 1260 1 7 3
 ATOM 628 CD1 LEU 80 -5.145 12.438 56.956 1.000 38.31
 ANISOU 628 CD1 LEU 80 5673 3891 4993 -1554 1987 -2 8 7
 ATOM 629 CD2 LEU 80 -3.137 13.884 57.306 1.000 29.85
 ANISOU 629 CD2 LEU 80 3502 3919 3920 125 1307 -2 6 4
 ATOM 630 N GLU 81 -6.853 12.055 60.396 1.000 25.58
 ANISOU 630 N GLU 81 2469 2759 4490 -196 -82 5 1 0
 ATOM 631 CA GLU 81 -6.739 11.038 61.415 1.000 25.98
 ANISOU 631 CA GLU 81 2739 2692 4441 -258 -55 4 2 4
 ATOM 632 C GLU 81 -5.299 10.536 61.562 1.000 26.28
 ANISOU 632 C GLU 81 2870 3268 3848 187 407 8 4 1
 ATOM 633 O GLU 81 -4.489 10.655 60.655 1.000 28.19
 ANISOU 633 O GLU 81 3709 3520 3483 253 799 -5 4 4
 ATOM 634 CB GLU 81 -7.685 9.861 61.123 1.000 29.83
 ANISOU 634 CB GLU 81 3533 2894 4906 -770 270 1 8 1
 ATOM 635 CG GLU 81 -7.241 8.832 60.098 1.000 25.34
 ANISOU 635 CG GLU 81 1737 2915 4976 284 -1220 1 5 8
 ATOM 636 CD GLU 81 -7.568 9.156 58.649 1.000 27.00
 ANISOU 636 CD GLU 81 1841 3405 5012 475 -1887 -4 5 6
 ATOM 637 OE1 GLU 81 -8.120 10.240 58.324 1.000 28.81
 ANISOU 637 OE1 GLU 81 3444 3091 4413 322 -155 7 9 1
 ATOM 638 OE2 GLU 81 -7.240 8.273 57.814 1.000 31.31
 ANISOU 638 OE2 GLU 81 3514 3384 4999 162 352 1 0 0
 ATOM 639 N SER 82 -4.988 9.974 62.720 1.000 31.00
 ANISOU 639 N SER 82 3568 3780 4430 -65 -30 1 4 8 4
 ATOM 640 CA SER 82 -3.653 9.422 62.959 1.000 30.29
 ANISOU 640 CA SER 82 3692 3278 4540 -157 -515 1 0 1 1
 ATOM 641 C SER 82 -3.421 8.150 62.150 1.000 31.76

- 111 -

ANISOU	641	C	SER	82	3995	3241	4831	-102	-1104	8 4 7
ATOM	642	O	SER	82	-4.313	7.728	61.397	1.000	34.01	
ANISOU	642	O	SER	82	3193	3794	5935	458	-1188	1 3 4
ATOM	643	CB	SER	82	-3.463	9.167	64.452	1.000	34.74	
ANISOU	643	CB	SER	82	4687	3907	4606	-232	-979	9 7 1
ATOM	644	OG	SER	82	-2.360	8.305	64.681	1.000	41.53	
ANISOU	644	OG	SER	82	4922	5366	5490	236	-1958	9 7 0
ATOM	645	N	GLY	91	-17.230	9.498	70.136	1.000	42.64	
ANISOU	645	N	GLY	91	4516	7599	4086	-2166	2340	-4 2 7
ATOM	646	CA	GLY	91	-17.485	10.892	69.789	1.000	44.91	
ANISOU	646	CA	GLY	91	6666	7702	2697	-4311	-1561	5 6 5
ATOM	647	C	GLY	91	-16.227	11.662	69.452	1.000	38.67	
ANISOU	647	C	GLY	91	5455	7587	1652	-2821	-274	-1 5 9
ATOM	648	O	GLY	91	-15.164	11.480	70.040	1.000	32.45	
ANISOU	648	O	GLY	91	4241	4474	3616	-183	1152	-4 3 9
ATOM	649	N	GLY	92	-16.332	12.558	68.474	1.000	31.97	
ANISOU	649	N	GLY	92	3881	5904	2363	-1382	735	-5 7 1
ATOM	650	CA	GLY	92	-15.232	13.412	68.075	1.000	33.02	
ANISOU	650	CA	GLY	92	4121	6150	2274	-1716	851	-9 5 6
ATOM	651	C	GLY	92	-15.223	13.696	66.572	1.000	26.22	
ANISOU	651	C	GLY	92	2603	5046	2314	-885	741	-9 4 7
ATOM	652	O	GLY	92	-16.289	13.666	65.939	1.000	23.91	
ANISOU	652	O	GLY	92	2490	3396	3198	-680	548	-5 6 7
ATOM	653	N	SER	93	-14.010	13.956	66.088	1.000	23.77	
ANISOU	653	N	SER	93	2405	3917	2708	-372	736	-5 6 0
ATOM	654	CA	SER	93	-13.801	14.287	64.690	1.000	23.41	
ANISOU	654	CA	SER	93	2700	3292	2901	-386	970	-3 9 9
ATOM	655	C	SER	93	-12.410	13.852	64.240	1.000	24.26	
ANISOU	655	C	SER	93	2547	3908	2763	-286	833	-2 2 4
ATOM	656	O	SER	93	-11.497	13.831	65.089	1.000	27.06	
ANISOU	656	O	SER	93	3401	3536	3346	630	92	-3 8 6
ATOM	657	CB	SER	93	-13.966	15.795	64.467	1.000	25.71	
ANISOU	657	CB	SER	93	2811	3225	3735	-576	271	-5 0 6
ATOM	658	OG	SER	93	-13.558	16.158	63.150	1.000	28.14	
ANISOU	658	OG	SER	93	2694	3713	4284	-373	290	5 1 7
ATOM	659	N	TYR	94	-12.254	13.533	62.949	1.000	24.24	
ANISOU	659	N	TYR	94	2786	3320	3104	-204	791	-8 1 7
ATOM	660	CA	TYR	94	-10.878	13.262	62.498	1.000	23.94	
ANISOU	660	CA	TYR	94	3089	2502	3505	95	1112	-6 8 3
ATOM	661	C	TYR	94	-10.017	14.531	62.584	1.000	25.19	
ANISOU	661	C	TYR	94	2601	2657	4312	147	737	-6 2 5
ATOM	662	O	TYR	94	-8.786	14.421	62.694	1.000	30.11	
ANISOU	662	O	TYR	94	2617	3095	5726	307	760	3 6
ATOM	663	CB	TYR	94	-10.800	12.659	61.098	1.000	25.64	
ANISOU	663	CB	TYR	94	3566	2910	3267	-293	1331	-5 2 5
ATOM	664	CG	TYR	94	-11.600	11.410	60.876	1.000	23.22	
ANISOU	664	CG	TYR	94	3359	2768	2697	-69	784	-2 7 4
ATOM	665	CD1	TYR	94	-12.451	11.455	59.777	1.000	26.01	
ANISOU	665	CD1	TYR	94	4410	2730	2741	499	353	-5 4 3
ATOM	666	CD2	TYR	94	-11.564	10.252	61.635	1.000	24.42	
ANISOU	666	CD2	TYR	94	3117	2866	3297	73	458	-1 4
ATOM	667	CE1	TYR	94	-13.243	10.407	59.443	1.000	28.75	
ANISOU	667	CE1	TYR	94	4559	3328	3037	434	140	-1 3 7 0
ATOM	668	CE2	TYR	94	-12.375	9.159	61.305	1.000	26.47	
ANISOU	668	CE2	TYR	94	4707	2585	2764	-220	1227	-7 1 8
ATOM	669	CZ	TYR	94	-13.209	9.247	60.212	1.000	29.70	
ANISOU	669	CZ	TYR	94	5641	3518	2125	-1172	1103	-1 4 4 7
ATOM	670	OH	TYR	94	-14.059	8.281	59.730	1.000	34.02	
ANISOU	670	OH	TYR	94	3079	3962	5886	-423	1593	-2 6 3 8
ATOM	671	N	SER	95	-10.628	15.714	62.561	1.000	22.61	
ANISOU	671	N	SER	95	2460	2497	3632	-54	59	-3 3 8

- 112 -

ATOM 672 CA SER 95 -9.924 16.975 62.750 1.000 22.54
 ANISOU 672 CA SER 95 2257 2603 3706 -120 -301 4 6
 ATOM 673 C SER 95 -9.370 17.106 64.163 1.000 23.58
 ANISOU 673 C SER 95 1811 3478 3671 -521 -88 -8 5
 ATOM 674 O SER 95 -8.623 18.034 64.481 1.000 26.53
 ANISOU 674 O SER 95 2592 3242 4247 -469 -167 -6 4 1
 ATOM 675 CB SER 95 -10.838 18.177 62.478 1.000 27.58
 ANISOU 675 CB SER 95 3657 2556 4264 365 -379 2 8
 ATOM 676 OG SER 95 -11.506 18.093 61.242 1.000 39.40
 ANISOU 676 OG SER 95 6336 4214 4421 900 -1445 1 4 4 2
 ATOM 677 N ASP 96 -9.712 16.194 65.060 1.000 25.04
 ANISOU 677 N ASP 96 2579 3688 3248 -399 277 -2 3 2
 ATOM 678 CA ASP 96 -9.228 16.317 66.422 1.000 24.42
 ANISOU 678 CA ASP 96 2603 3347 3330 -470 257 -5 2 6
 ATOM 679 C ASP 96 -7.735 16.050 66.501 1.000 24.45
 ANISOU 679 C ASP 96 2597 3228 3466 -471 162 -3 8 3
 ATOM 680 O ASP 96 -7.073 16.589 67.404 1.000 26.51
 ANISOU 680 O ASP 96 2656 4047 3370 -170 160 -7 9 8
 ATOM 681 CB ASP 96 -9.952 15.334 67.334 1.000 24.97
 ANISOU 681 CB ASP 96 2310 3806 3371 -423 -228 7 7
 ATOM 682 CG ASP 96 -11.411 15.605 67.606 1.000 26.77
 ANISOU 682 CG ASP 96 2272 4334 3566 -362 -240 7 1 6
 ATOM 683 OD1 ASP 96 -11.935 16.723 67.388 1.000 33.94
 ANISOU 683 OD1 ASP 96 3267 4894 4733 647 204 5 6 9
 ATOM 684 OD2 ASP 96 -12.058 14.646 68.083 1.000 32.65
 ANISOU 684 OD2 ASP 96 3624 4709 4072 -1032 1446 -2 0 2
 ATOM 685 N TYR 97 -7.254 15.226 65.581 1.000 22.21
 ANISOU 685 N TYR 97 2292 3389 2760 -376 -77 -1 0 2
 ATOM 686 CA TYR 97 -5.835 14.852 65.583 1.000 23.71
 ANISOU 686 CA TYR 97 2480 3542 2987 -27 106 6 4 4
 ATOM 687 C TYR 97 -5.026 15.828 64.743 1.000 23.06
 ANISOU 687 C TYR 97 2363 3754 2647 -410 -78 3 5 0
 ATOM 688 O TYR 97 -3.992 16.327 65.230 1.000 24.29
 ANISOU 688 O TYR 97 2205 3845 3178 -133 -230 7 4
 ATOM 689 CB TYR 97 -5.585 13.451 65.035 1.000 28.38
 ANISOU 689 CB TYR 97 3230 3324 4229 540 -450 8 3 2
 ATOM 690 CG TYR 97 -4.132 13.025 65.082 1.000 30.37
 ANISOU 690 CG TYR 97 3278 4101 4161 766 -191 6 7 1
 ATOM 691 CD1 TYR 97 -3.511 12.691 66.285 1.000 30.19
 ANISOU 691 CD1 TYR 97 2878 4475 4119 1106 151 9 5 1
 ATOM 692 CD2 TYR 97 -3.370 12.945 63.922 1.000 29.79
 ANISOU 692 CD2 TYR 97 3317 4005 3997 53 -253 5 4 4
 ATOM 693 CE1 TYR 97 -2.178 12.294 66.324 1.000 32.77
 ANISOU 693 CE1 TYR 97 2554 4771 5126 574 -68 7 6 3
 ATOM 694 CE2 TYR 97 -2.043 12.553 63.955 1.000 32.68
 ANISOU 694 CE2 TYR 97 3536 3793 5087 403 353 3 2 3
 ATOM 695 CZ TYR 97 -1.445 12.228 65.157 1.000 33.00
 ANISOU 695 CZ TYR 97 2633 4284 5622 1066 264 4 5 6
 ATOM 696 OH TYR 97 -0.121 11.845 65.156 1.000 42.66
 ANISOU 696 OH TYR 97 2572 5373 8264 1161 764 1 2 7 7
 ATOM 697 CB SER 98 -3.465 16.575 62.134 1.000 23.20
 ANISOU 697 CB SER 98 2461 2766 3587 105 2 -5 4 4
 ATOM 698 OG SER 98 -3.632 15.649 61.078 1.000 26.49
 ANISOU 698 OG SER 98 3824 3059 3180 -154 238 -4 5 7
 ATOM 699 C SER 98 -5.694 17.744 61.701 1.000 18.66
 ANISOU 699 C SER 98 2301 2150 2637 -295 66 1 3
 ATOM 700 O SER 98 -6.768 17.212 61.413 1.000 20.88
 ANISOU 700 O SER 98 3042 2245 2646 -945 -249 1 8 1
 ATOM 701 N SER 98 -5.457 16.110 63.511 1.000 23.62
 ANISOU 701 N SER 98 2816 3227 2931 -441 -395 6 0 5
 ATOM 702 CA SER 98 -4.748 17.143 62.741 1.000 21.31

- 113 -

ANISOU 702	CA	SER	98	2430	2687	2982	133	153	2 9 4
ATOM 703	N	MET	99	-5.307	18.891	61.148	1.000	18.68	
ANISOU 703	N	MET	99	2392	2722	1984	-978	-366	1 0 1
ATOM 704	CA	MET	99	-6.047	19.560	60.075	1.000	17.84	
ANISOU 704	CA	MET	99	2431	2620	1726	-945	-212	- 1 7
ATOM 705	CB	MET	99	-6.819	20.779	60.585	1.000	19.71	
ANISOU 705	CB	MET	99	2348	2968	2173	-679	25 6 4	
ATOM 706	CG	MET	99	-8.052	20.392	61.374	1.000	23.68	
ANISOU 706	CG	MET	99	2360	3055	3582	-504	393	4 8 9
ATOM 707	SD	MET	99	-9.031	21.821	61.911	1.000	22.33	
ANISOU 707	SD	MET	99	2569	3383	2534	-522	170	- 1 2 0
ATOM 708	CE	MET	99	-8.148	22.225	63.419	1.000	36.98	
ANISOU 708	CE	MET	99	6485	4165	3401	-225	-1904	- 2 3
ATOM 709	C	MET	99	-5.070	19.954	58.973	1.000	17.19	
ANISOU 709	C	MET	99	2269	2488	1776	-960	-194	- 2 0 1
ATOM 710	O	MET	99	-3.964	20.341	59.324	1.000	16.93	
ANISOU 710	O	MET	99	1932	2583	1919	-367	-208	- 2 4 1
ATOM 711	N	CYS	100	-5.486	19.864	57.715	1.000	20.00	
ANISOU 711	N	CYS	100	3178	2683	1739	-1753	-358	1 6 6
ATOM 712	CA	CYS	100	-4.645	20.181	56.554	1.000	16.64	
ANISOU 712	CA	CYS	100	2213	2294	1817	-924	-563	4 6 8
ATOM 713	CB	CYS	100	-4.291	18.893	55.813	1.000	17.74	
ANISOU 713	CB	CYS	100	2161	2174	2407	560	-765	1 0 5 3
ATOM 714	SG	CYS	100	-3.035	18.928	54.552	1.000	33.56	
ANISOU 714	SG	CYS	100	5244	3511	3997	414	1509	6 0 1
ATOM 715	C	CYS	100	-5.347	21.121	55.590	1.000	13.48	
ANISOU 715	C	CYS	100	1879	1415	1829	-68	240	- 9 1
ATOM 716	O	CYS	100	-6.585	21.127	55.496	1.000	14.49	
ANISOU 716	O	CYS	100	1880	1952	1673	-497	-57	1 4
ATOM 717	N	TYR	101	-4.589	21.921	54.852	1.000	13.35	
ANISOU 717	N	TYR	101	1721	1677	1673	-254	-78	4 9
ATOM 718	CA	TYR	101	-5.016	22.753	53.755	1.000	10.27	
ANISOU 718	CA	TYR	101	926 1498	1477	-15	-141	- 2 3 1	
ATOM 719	CB	TYR	101	-5.102	24.265	54.124	1.000	13.60	
ANISOU 719	CB	TYR	101	1626	1513	2027	-48	322	- 2 3 6
ATOM 720	CG	TYR	101	-5.498	25.025	52.863	1.000	17.31	
ANISOU 720	CG	TYR	101	2373	1509	2694	-158	-103	1 9 3
ATOM 721	CD1	TYR	101	-6.815	25.068	52.519	1.000	16.38	
ANISOU 721	CD1	TYR	101	2464	752 3006	190	-227	5 5	
ATOM 722	CE1	TYR	101	-7.307	25.715	51.412	1.000	17.01	
ANISOU 722	CE1	TYR	101	2755	714 2993	-86	-416	1 2 2	
ATOM 723	CD2	TYR	101	-4.616	25.679	52.012	1.000	19.51	
ANISOU 723	CD2	TYR	101	3032	1533	2847	-1143	-594	4 7 5
ATOM 724	CE2	TYR	101	-5.065	26.321	50.872	1.000	20.96	
ANISOU 724	CE2	TYR	101	2802	1949	3211	238	112	7 6 9
ATOM 725	CZ	TYR	101	-6.414	26.334	50.568	1.000	22.78	
ANISOU 725	CZ	TYR	101	3238	2291	3126	-1228	-919	6 2 4
ATOM 726	OH	TYR	101	-6.875	26.986	49.442	1.000	23.10	
ANISOU 726	OH	TYR	101	3141	3112	2522	-14	-129	4 2 9
ATOM 727	C	TYR	101	-4.041	22.518	52.596	1.000	11.25	
ANISOU 727	C	TYR	101	1223	1398	1654	-323	103	- 2 5 2
ATOM 728	O	TYR	101	-2.823	22.677	52.787	1.000	12.23	
ANISOU 728	O	TYR	101	1114	1750	1784	-87	130	- 2 0
ATOM 729	N	SER	102	-4.542	22.190	51.405	1.000	11.17	
ANISOU 729	N	SER	102	1355	1279	1611	-220	145	- 2 6 3
ATOM 730	CA	SER	102	-3.752	21.802	50.235	1.000	10.46	
ANISOU 730	CA	SER	102	1144	1263	1568	62 -1	-125	
ATOM 731	CB	SER	102	-4.027	20.343	49.908	1.000	13.46	
ANISOU 731	CB	SER	102	1668	1212	2234	324	105	- 3 0 1
ATOM 732	OG	SER	102	-3.723	19.487	51.025	1.000	16.42	
ANISOU 732	OG	SER	102	2291	1313	2637	-122	-43	9 6

- 114 -

ATOM	733	C	SER	102	-4.046	22.668	49.008	1.000	11.74	
ANISOU	733	C	SER	102	1346	1500	1614	18	-39	-10
ATOM	734	O	SER	102	-5.148	23.148	48.784	1.000	12.84	
ANISOU	734	O	SER	102	1480	1410	1988	90	-66	249
ATOM	735	N	MET	103	-3.004	22.871	48.187	1.000	12.33	
ANISOU	735	N	MET	103	1554	1722	1409	-262	-10	-246
ATOM	736	CA	MET	103	-3.188	23.603	46.938	1.000	12.92	
ANISOU	736	CA	MET	103	1663	1681	1565	22	47	-70
ATOM	737	CB	MET	103	-3.215	25.122	47.179	1.000	17.51	
ANISOU	737	CB	MET	103	2439	1634	2579	-363	812	-44
ATOM	738	CG	MET	103	-1.929	25.808	47.549	1.000	20.07	
ANISOU	738	CG	MET	103	2509	1470	3646	-538	688	376
ATOM	739	SD	MET	103	-2.136	27.614	47.689	1.000	18.10	
ANISOU	739	SD	MET	103	2235	1665	2975	-3	-334	-352
ATOM	740	CE	MET	103	-2.365	28.068	45.991	1.000	18.09	
ANISOU	740	CE	MET	103	2319	1457	3098	-187	-718	-214
ATOM	741	C	MET	103	-2.152	23.221	45.892	1.000	12.57	
ANISOU	741	C	MET	103	1420	1837	1519	119	-53	238
ATOM	742	O	MET	103	-1.120	22.573	46.175	1.000	12.57	
ANISOU	742	O	MET	103	1094	1891	1792	-155	-165	276
ATOM	743	N	GLY	104	-2.418	23.650	44.655	1.000	12.83	
ANISOU	743	N	GLY	104	1493	1958	1422	237	-124	-34
ATOM	744	CA	GLY	104	-1.533	23.459	43.513	1.000	12.65	
ANISOU	744	CA	GLY	104	1075	2188	1544	-93	-37	242
ATOM	745	C	GLY	104	-1.624	24.622	42.542	1.000	14.36	
ANISOU	745	C	GLY	104	1909	1985	1561	-265	-294	142
ATOM	746	O	GLY	104	-2.033	25.700	42.967	1.000	15.69	
ANISOU	746	O	GLY	104	1628	2273	2060	163	-197	213
ATOM	747	N	THR	105	-1.242	24.397	41.276	1.000	14.52	
ANISOU	747	N	THR	105	1829	2182	1504	-59	-375	319
ATOM	748	CA	THR	105	-1.218	25.452	40.279	1.000	15.27	
ANISOU	748	CA	THR	105	1977	2223	1603	-105	-363	365
ATOM	749	CB	THR	105	-0.359	25.083	39.039	1.000	15.61	
ANISOU	749	CB	THR	105	1936	2122	1873	-37	-106	554
ATOM	750	OG1	THR	105	-0.884	23.876	38.446	1.000	16.16	
ANISOU	750	OG1	THR	105	1738	2260	2140	217	-285	151
ATOM	751	CG2	THR	105	1.092	24.882	39.369	1.000	17.47	
ANISOU	751	CG2	THR	105	1918	2871	1847	-293	-227	527
ATOM	752	C	THR	105	-2.603	25.828	39.755	1.000	14.73	
ANISOU	752	C	THR	105	1989	1694	1913	122	-340	199
ATOM	753	O	THR	105	-2.730	26.921	39.174	1.000	19.91	
ANISOU	753	O	THR	105	2579	2355	2632	23	-437	1004
ATOM	754	N	ALA	106	-3.587	24.960	39.913	1.000	16.57	
ANISOU	754	N	ALA	106	1836	2413	2047	2	-260	661
ATOM	755	CA	ALA	106	-4.975	25.167	39.465	1.000	14.94	
ANISOU	755	CA	ALA	106	1975	1904	1798	105	-456	365
ATOM	756	CB	ALA	106	-5.054	24.945	37.965	1.000	17.75	
ANISOU	756	CB	ALA	106	2006	2862	1876	140	-201	-32
ATOM	757	C	ALA	106	-5.942	24.251	40.222	1.000	16.26	
ANISOU	757	C	ALA	106	1710	2174	2293	327	-127	491
ATOM	758	O	ALA	106	-5.498	23.398	41.013	1.000	14.57	
ANISOU	758	O	ALA	106	1622	1971	1945	213	-21	337
ATOM	759	N	ASP	107	-7.253	24.410	40.008	1.000	16.71	
ANISOU	759	N	ASP	107	1768	2096	2485	540	-22	304
ATOM	760	CA	ASP	107	-8.310	23.638	40.633	1.000	16.10	
ANISOU	760	CA	ASP	107	1696	2175	2246	51	-485	-14
ATOM	761	CB	ASP	107	-8.231	22.171	40.211	1.000	17.09	
ANISOU	761	CB	ASP	107	1299	2385	2808	144	-203	-399
ATOM	762	CG	ASP	107	-8.418	21.966	38.720	1.000	21.54	
ANISOU	762	CG	ASP	107	2385	2894	2906	84	-317	-722
ATOM	763	OD1	ASP	107	-9.452	22.445	38.189	1.000	23.92	

- 115 -

ANISOU 763	OD1	ASP	107	3447	2970	2672	698	-753	-772
ATOM 764	OD2	ASP	107	-7.563	21.311	38.080	1.000	24.88	
ANISOU 764	OD2	ASP	107	2496	4004	2954	105	244	-679
ATOM 765	C	ASP	107	-8.285	23.785	42.160	1.000	14.16	
ANISOU 765	C	ASP	107	1261	1918	2201	237	-447	153
ATOM 766	O	ASP	107	-8.507	22.850	42.936	1.000	16.67	
ANISOU 766	O	ASP	107	2017	1927	2390	-189	-193	97
ATOM 767	N	ASN	108	-8.027	25.020	42.598	1.000	15.34	
ANISOU 767	N	ASN	108	2093	1866	1870	82	51	239
ATOM 768	CA	ASN	108	-7.967	25.314	44.031	1.000	13.68	
ANISOU 768	CA	ASN	108	1479	1823	1898	153	107	257
ATOM 769	CB	ASN	108	-6.925	26.420	44.272	1.000	15.60	
ANISOU 769	CB	ASN	108	1593	2026	2309	16	267	-98
ATOM 770	CG	ASN	108	-5.516	25.942	43.963	1.000	15.23	
ANISOU 770	CG	ASN	108	1505	2141	2142	5	-53	2
ATOM 771	OD1	ASN	108	-5.086	24.932	44.505	1.000	15.40	
ANISOU 771	OD1	ASN	108	1412	2442	1998	-5	-239	188
ATOM 772	ND2	ASN	108	-4.823	26.678	43.094	1.000	16.96	
ANISOU 772	ND2	ASN	108	1593	2198	2652	339	393	222
ATOM 773	C	ASN	108	-9.310	25.708	44.642	1.000	14.55	
ANISOU 773	C	ASN	108	1471	1937	2120	261	191	526
ATOM 774	O	ASN	108	-10.222	26.170	43.958	1.000	16.89	
ANISOU 774	O	ASN	108	1861	2336	2219	716	-109	14
ATOM 775	N	LEU	109	-9.412	25.512	45.954	1.000	13.42	
ANISOU 775	N	LEU	109	1458	1648	1994	179	130	9
ATOM 776	CA	LEU	109	-10.602	25.796	46.769	1.000	13.53	
ANISOU 776	CA	LEU	109	1094	2122	1923	-52	-86	-256
ATOM 777	CB	LEU	109	-11.187	24.499	47.331	1.000	14.50	
ANISOU 777	CB	LEU	109	1382	1959	2169	119	455	-468
ATOM 778	CG	LEU	109	-11.580	23.383	46.370	1.000	15.21	
ANISOU 778	CG	LEU	109	1593	1785	2403	235	63	-342
ATOM 779	CD1	LEU	109	-11.931	22.083	47.089	1.000	18.26	
ANISOU 779	CD1	LEU	109	2460	1674	2806	382	-414	-94
ATOM 780	CD2	LEU	109	-12.780	23.783	45.529	1.000	22.36	
ANISOU 780	CD2	LEU	109	3055	2391	3052	44	-1155	288
ATOM 781	C	LEU	109	-10.203	26.794	47.840	1.000	13.54	
ANISOU 781	C	LEU	109	1179	1989	1979	76	-116	-259
ATOM 782	O	LEU	109	-9.416	26.428	48.717	1.000	16.15	
ANISOU 782	O	LEU	109	2196	2210	1730	-52	-366	32
ATOM 783	N	PHE	110	-10.706	28.025	47.786	1.000	16.11	
ANISOU 783	N	PHE	110	1369	2042	2709	105	-118	-288
ATOM 784	CA	PHE	110	-10.298	29.079	48.732	1.000	17.05	
ANISOU 784	CA	PHE	110	1626	1801	3050	-116	259	-362
ATOM 785	CB	PHE	110	-9.660	30.259	47.991	1.000	17.94	
ANISOU 785	CB	PHE	110	1423	2366	3027	-290	228	-129
ATOM 786	CG	PHE	110	-8.425	29.972	47.165	1.000	20.32	
ANISOU 786	CG	PHE	110	1702	2650	3368	-176	459	-385
ATOM 787	CD1	PHE	110	-7.257	29.598	47.793	1.000	20.35	
ANISOU 787	CD1	PHE	110	1885	2462	3387	461	573	-707
ATOM 788	CD2	PHE	110	-8.405	30.110	45.789	1.000	20.31	
ANISOU 788	CD2	PHE	110	2073	2226	3419	512	712	-264
ATOM 789	CE1	PHE	110	-6.102	29.347	47.065	1.000	19.49	
ANISOU 789	CE1	PHE	110	1958	2116	3332	176	749	-631
ATOM 790	CE2	PHE	110	-7.288	29.846	45.050	1.000	20.65	
ANISOU 790	CE2	PHE	110	2158	2094	3596	758	724	-321
ATOM 791	CZ	PHE	110	-6.118	29.496	45.694	1.000	19.43	
ANISOU 791	CZ	PHE	110	1925	2131	3327	219	542	-780
ATOM 792	C	PHE	110	-11.495	29.556	49.538	1.000	17.08	
ANISOU 792	C	PHE	110	1774	1806	2911	-74	414	-111
ATOM 793	O	PHE	110	-12.562	29.792	48.929	1.000	21.26	
ANISOU 793	O	PHE	110	1849	2577	3650	405	178	-448

- 116 -

ATOM	794	N	PRO	111	-11.406	29.717	50.851	1.000	19.41	
ANISOU	794	N	PRO	111	2279	2110	2985	-386	519	-314
ATOM	795	CD	PRO	111	-10.278	29.322	51.705	1.000	19.20	
ANISOU	795	CD	PRO	111	2773	1880	2640	-417	255	-514
ATOM	796	CA	PRO	111	-12.549	30.252	51.604	1.000	21.47	
ANISOU	796	CA	PRO	111	3026	1924	3206	-50	728	-635
ATOM	797	CB	PRO	111	-12.167	30.007	53.055	1.000	23.63	
ANISOU	797	CB	PRO	111	3789	2054	3137	334	776	-575
ATOM	798	CG	PRO	111	-10.775	29.535	53.100	1.000	22.33	
ANISOU	798	CG	PRO	111	2767	2908	2809	-1006	623	-414
ATOM	799	C	PRO	111	-12.828	31.739	51.433	1.000	23.88	
ANISOU	799	C	PRO	111	3139	2049	3887	79	-142	-479
ATOM	800	O	PRO	111	-13.919	32.194	51.834	1.000	26.77	
ANISOU	800	O	PRO	111	3800	2818	3555	992	-91	-397
ATOM	801	N	SER	112	-11.906	32.517	50.872	1.000	25.19	
ANISOU	801	N	SER	112	3514	2269	3788	-247	-856	282
ATOM	802	CA	SER	112	-12.300	33.919	50.631	1.000	26.43	
ANISOU	802	CA	SER	112	2654	2655	4734	496	1364	456
ATOM	803	CB	SER	112	-12.506	34.712	51.912	1.000	33.37	
ANISOU	803	CB	SER	112	3122	3663	5895	172	2582	-510
ATOM	804	OG	SER	112	-11.322	34.719	52.688	1.000	36.94	
ANISOU	804	OG	SER	112	6530	2154	5351	1399	206	-415
ATOM	805	C	SER	112	-11.262	34.587	49.723	1.000	26.62	
ANISOU	805	C	SER	112	2613	2546	4956	1021	1668	651
ATOM	806	O	SER	112	-10.219	34.029	49.414	1.000	22.81	
ANISOU	806	O	SER	112	2241	2782	3645	800	837	-400
ATOM	807	N	GLY	113	-11.570	35.802	49.279	1.000	28.93	
ANISOU	807	N	GLY	113	2937	2947	5108	1008	1175	1198
ATOM	808	CA	GLY	113	-10.659	36.478	48.365	1.000	30.79	
ANISOU	808	CA	GLY	113	2992	3606	5102	381	798	1400
ATOM	809	C	GLY	113	-9.362	36.829	49.070	1.000	31.83	
ANISOU	809	C	GLY	113	3297	3919	4878	262	897	528
ATOM	810	O	GLY	113	-8.294	36.790	48.459	1.000	25.85	
ANISOU	810	O	GLY	113	2920	2317	4585	857	450	-203
ATOM	811	N	ASP	114	-9.479	37.145	50.365	1.000	29.56	
ANISOU	811	N	ASP	114	3487	2877	4868	866	1104	760
ATOM	812	CA	ASP	114	-8.257	37.463	51.122	1.000	26.15	
ANISOU	812	CA	ASP	114	3189	2680	4066	1028	1584	542
ATOM	813	CB	ASP	114	-8.628	37.937	52.526	1.000	33.81	
ANISOU	813	CB	ASP	114	5580	2697	4569	1774	1691	-240
ATOM	814	CG	ASP	114	-7.904	39.232	52.840	1.000	40.77	
ANISOU	814	CG	ASP	114	6798	3734	4960	719	693	-248
ATOM	815	OD1	ASP	114	-8.330	40.277	52.295	1.000	48.61	
ANISOU	815	OD1	ASP	114	6014	2534	9920	1703	931	-913
ATOM	816	OD2	ASP	114	-6.932	39.178	53.622	1.000	54.35	
ANISOU	816	OD2	ASP	114	5258	7609	7783	-868	495	1602
ATOM	817	C	ASP	114	-7.310	36.281	51.231	1.000	23.05	
ANISOU	817	C	ASP	114	2621	2102	4033	444	1874	340
ATOM	818	O	ASP	114	-6.111	36.371	50.955	1.000	22.05	
ANISOU	818	O	ASP	114	2423	2277	3677	131	1411	-461
ATOM	819	N	PHE	115	-7.854	35.160	51.637	1.000	23.21	
ANISOU	819	N	PHE	115	2945	1890	3984	-130	1293	-228
ATOM	820	CA	PHE	115	-7.120	33.896	51.690	1.000	19.93	
ANISOU	820	CA	PHE	115	2562	1908	3102	-198	655	-294
ATOM	821	CB	PHE	115	-8.085	32.792	52.157	1.000	19.49	
ANISOU	821	CB	PHE	115	2378	1754	3275	64	881	-314
ATOM	822	CG	PHE	115	-7.523	31.445	52.540	1.000	17.25	
ANISOU	822	CG	PHE	115	2053	1589	2912	-56	348	-695
ATOM	823	CD1	PHE	115	-7.637	30.951	53.833	1.000	19.00	
ANISOU	823	CD1	PHE	115	2728	1539	2950	73	496	-683
ATOM	824	CD2	PHE	115	-6.868	30.634	51.615	1.000	17.88	

- 117 -

ANISOU 824	CD2	PHE	115	1933	1931	2927	7	298	-810
ATOM 825	CE1	PHE	115	-7.100	29.711	54.163	1.000	20.25	
ANISOU 825	CE1	PHE	115	2825	1825	3042	317	341	-575
ATOM 826	CE2	PHE	115	-6.338	29.412	51.955	1.000	19.11	
ANISOU 826	CE2	PHE	115	1865	2158	3237	336	351	-885
ATOM 827	CZ	PHE	115	-6.452	28.936	53.233	1.000	19.39	
ANISOU 827	CZ	PHE	115	2068	1910	3390	320	248	-669
ATOM 828	C	PHE	115	-6.506	33.624	50.327	1.000	17.86	
ANISOU 828	C	PHE	115	1964	1945	2878	61	344	16
ATOM 829	O	PHE	115	-5.324	33.315	50.271	1.000	17.34	
ANISOU 829	O	PHE	115	1868	2107	2613	-132	179	157
ATOM 830	N	GLU	116	-7.310	33.683	49.263	1.000	18.21	
ANISOU 830	N	GLU	116	1921	1934	3065	547	281	62
ATOM 831	CA	GLU	116	-6.848	33.387	47.907	1.000	19.99	
ANISOU 831	CA	GLU	116	2128	2618	2851	81	231	222
ATOM 832	CB	GLU	116	-7.968	33.605	46.884	1.000	18.61	
ANISOU 832	CB	GLU	116	2058	1952	3060	231	244	270
ATOM 833	CG	GLU	116	-7.398	33.378	45.482	1.000	18.61	
ANISOU 833	CG	GLU	116	1813	2288	2971	295	-32	-33
ATOM 834	CD	GLU	116	-8.442	33.230	44.412	1.000	22.40	
ANISOU 834	CD	GLU	116	1908	3193	3410	-122	-278	-91
ATOM 835	OE1	GLU	116	-9.654	33.272	44.678	1.000	30.82	
ANISOU 835	OE1	GLU	116	1793	4465	5452	273	-414	-24
ATOM 836	OE2	GLU	116	-8.085	33.063	43.225	1.000	30.24	
ANISOU 836	OE2	GLU	116	3333	5132	3026	382	-658	327
ATOM 837	C	GLU	116	-5.620	34.211	47.535	1.000	18.82	
ANISOU 837	C	GLU	116	2090	2069	2990	294	119	487
ATOM 838	O	GLU	116	-4.605	33.701	47.049	1.000	17.41	
ANISOU 838	O	GLU	116	2228	1780	2606	45	259	282
ATOM 839	N	ARG	117	-5.660	35.508	47.777	1.000	21.02	
ANISOU 839	N	ARG	117	2313	2185	3487	408	220	90
ATOM 840	CA	ARG	117	-4.560	36.420	47.431	1.000	21.35	
ANISOU 840	CA	ARG	117	2337	1800	3976	466	147	-31
ATOM 841	C	ARG	117	-3.291	36.054	48.192	1.000	20.52	
ANISOU 841	C	ARG	117	2292	2124	3380	353	288	-10
ATOM 842	O	ARG	117	-2.186	35.969	47.636	1.000	18.96	
ANISOU 842	O	ARG	117	2223	1664	3316	138	318	231
ATOM 843	CB	ARG	117	-4.971	37.885	47.693	1.000	25.59	
ANISOU 843	CB	ARG	117	3237	1900	4587	929	1882	632
ATOM 844	CG	ARG	117	-3.881	38.908	47.478	1.000	32.57	
ANISOU 844	CG	ARG	117	5212	1925	5237	-281	1083	623
ATOM 845	CD	ARG	117	-4.325	40.323	47.859	1.000	36.56	
ANISOU 845	CD	ARG	117	6009	2157	5724	149	1774	663
ATOM 846	NE	ARG	117	-5.162	40.335	49.056	1.000	44.43	
ANISOU 846	NE	ARG	117	7200	3742	5940	-96	2344	-15
ATOM 847	CZ	ARG	117	-4.763	40.501	50.306	1.000	45.48	
ANISOU 847	CZ	ARG	117	6422	4804	6054	-370	2388	-283
ATOM 848	NH1	ARG	117	-3.484	40.683	50.619	1.000	53.21	
ANISOU 848	NH1	ARG	117	6867	6451	6900	-2543	2487	354
ATOM 849	NH2	ARG	117	-5.647	40.487	51.301	1.000	50.00	
ANISOU 849	NH2	ARG	117	6265	6511	6220	224	2433	-1534
ATOM 850	N	ILE	118	-3.439	35.832	49.493	1.000	19.30	
ANISOU 850	N	ILE	118	2275	1838	3221	128	407	-645
ATOM 851	CA	ILE	118	-2.275	35.527	50.331	1.000	18.25	
ANISOU 851	CA	ILE	118	2376	1745	2811	78	530	-449
ATOM 852	CB	ILE	118	-2.665	35.597	51.820	1.000	18.24	
ANISOU 852	CB	ILE	118	2201	1726	3003	346	906	-306
ATOM 853	CG2	ILE	118	-1.712	34.851	52.732	1.000	18.49	
ANISOU 853	CG2	ILE	118	2077	2158	2792	-202	308	-530
ATOM 854	CG1	ILE	118	-2.877	37.031	52.368	1.000	24.69	
ANISOU 854	CG1	ILE	118	4436	1808	3136	284	1382	-414

- 118 -

ATOM	855	CD1	ILE	118	-3.786	37.025	53.582	1.000	29.63
ANISOU	855	CD1	ILE	118	6169	3096	1994	189	1258 -1068
ATOM	856	C	ILE	118	-1.692	34.172	49.959	1.000	15.65
ANISOU	856	C	ILE	118	2316	1549	2082	-89	573 -117
ATOM	857	O	ILE	118	-0.463	34.035	49.802	1.000	14.59
ANISOU	857	O	ILE	118	2240	1255	2051	16	286 214
ATOM	858	N	TRP	119	-2.523	33.139	49.784	1.000	14.44
ANISOU	858	N	TRP	119	2125	1592	1771	47	128 -71
ATOM	859	CA	TRP	119	-2.010	31.795	49.518	1.000	13.68
ANISOU	859	CA	TRP	119	1712	1529	1957	-61	220 40
ATOM	860	CB	TRP	119	-3.089	30.755	49.932	1.000	14.93
ANISOU	860	CB	TRP	119	1819	1729	2123	-234	295 -35
ATOM	861	CG	TRP	119	-2.864	30.482	51.420	1.000	16.19
ANISOU	861	CG	TRP	119	1640	2364	2146	-168	582 167
ATOM	862	CD2	TRP	119	-2.116	29.430	51.993	1.000	20.41
ANISOU	862	CD2	TRP	119	3189	2414	2151	202	523 405
ATOM	863	CE2	TRP	119	-2.177	29.580	53.392	1.000	19.84
ANISOU	863	CE2	TRP	119	3536	1818	2184	-439	234 137
ATOM	864	CE3	TRP	119	-1.390	28.357	51.456	1.000	23.94
ANISOU	864	CE3	TRP	119	5382	1647	2068	561	126 400
ATOM	865	CD1	TRP	119	-3.340	31.223	52.460	1.000	20.05
ANISOU	865	CD1	TRP	119	3207	2343	2069	-9	189 -139
ATOM	866	NE1	TRP	119	-2.938	30.689	53.649	1.000	20.32
ANISOU	866	NE1	TRP	119	2806	2726	2188	-96	-68 -185
ATOM	867	CZ2	TRP	119	-1.547	28.714	54.281	1.000	22.12
ANISOU	867	CZ2	TRP	119	4071	2256	2078	-17	105 22
ATOM	868	CZ3	TRP	119	-0.761	27.490	52.332	1.000	21.52
ANISOU	868	CZ3	TRP	119	4214	2168	1794	311	-193 197
ATOM	869	CH2	TRP	119	-0.847	27.674	53.715	1.000	24.34
ANISOU	869	CH2	TRP	119	5349	2047	1850	329	148 183
ATOM	870	C	TRP	119	-1.521	31.634	48.095	1.000	14.27
ANISOU	870	C	TRP	119	2180	1259	1985	-187	334 -65
ATOM	871	O	TRP	119	-0.569	30.865	47.855	1.000	14.73
ANISOU	871	O	TRP	119	1996	1653	1946	-67	362 101
ATOM	872	N	THR	120	-2.109	32.325	47.116	1.000	13.99
ANISOU	872	N	THR	120	2231	1237	1848	106	627 -137
ATOM	873	CA	THR	120	-1.541	32.275	45.762	1.000	15.19
ANISOU	873	CA	THR	120	1903	2093	1774	9	435 -242
ATOM	874	CB	THR	120	-2.492	32.983	44.787	1.000	16.41
ANISOU	874	CB	THR	120	1934	2304	1995	-331	152 66
ATOM	875	OG1	THR	120	-3.738	32.297	44.766	1.000	18.53
ANISOU	875	OG1	THR	120	1891	2288	2863	-236	195 407
ATOM	876	CG2	THR	120	-1.974	32.906	43.358	1.000	18.02
ANISOU	876	CG2	THR	120	2135	2602	2108	324	322 318
ATOM	877	C	THR	120	-0.145	32.870	45.727	1.000	14.19
ANISOU	877	C	THR	120	1868	2050	1475	87	285 -167
ATOM	878	O	THR	120	0.756	32.299	45.078	1.000	13.62
ANISOU	878	O	THR	120	1864	1692	1620	301	354 217
ATOM	879	N	GLN	121	0.114	33.962	46.429	1.000	14.55
ANISOU	879	N	GLN	121	1721	1672	2136	304	175 -67
ATOM	880	CA	GLN	121	1.459	34.548	46.483	1.000	15.80
ANISOU	880	CA	GLN	121	2067	1666	2271	-18	-119 362
ATOM	881	C	GLN	121	2.465	33.642	47.176	1.000	13.73
ANISOU	881	C	GLN	121	1747	1665	1806	-30	18 114
ATOM	882	O	GLN	121	3.603	33.452	46.685	1.000	15.36
ANISOU	882	O	GLN	121	2063	1688	2084	48	360 -44
ATOM	883	CB	GLN	121	1.315	35.918	47.154	1.000	18.85
ANISOU	883	CB	GLN	121	2537	1426	3200	-73	-5 356
ATOM	884	CG	GLN	121	2.639	36.558	47.543	1.000	18.88
ANISOU	884	CG	GLN	121	2507	1788	2878	59	9 -248
ATOM	885	CD	GLN	121	3.468	36.936	46.337	1.000	20.70

- 119 -

ANISOU 885	CD	GLN	121	2584	2138	3142	-373	-85	2 3 1
ATOM 886	OE1	GLN	121	2.935	37.088	45.224	1.000	22.47	
ANISOU 886	OE1	GLN	121	2695	2822	3019	-245	0	1 2 1
ATOM 887	NE2	GLN	121	4.779	37.101	46.522	1.000	25.22	
ANISOU 887	NE2	GLN	121	2426	3344	3811	127	-131	1 3 8 5
ATOM 888	N	TYR	122	2.081	33.054	48.299	1.000	12.26	
ANISOU 888	N	TYR	122	1747	1514	1399	99	-55	-2 5 8
ATOM 889	CA	TYR	122	2.896	32.102	49.050	1.000	13.18	
ANISOU 889	CA	TYR	122	1901	1643	1464	-20	-253	-1 6 0
ATOM 890	CB	TYR	122	2.211	31.724	50.364	1.000	13.78	
ANISOU 890	CB	TYR	122	2045	1435	1756	116	48	-2 8
ATOM 891	CG	TYR	122	2.994	30.808	51.282	1.000	14.22	
ANISOU 891	CG	TYR	122	1966	1681	1758	101	68	1 0 1
ATOM 892	CD1	TYR	122	4.271	31.120	51.722	1.000	17.48	
ANISOU 892	CD1	TYR	122	1788	1972	2882	149	-5	4 2 0
ATOM 893	CE1	TYR	122	5.003	30.284	52.576	1.000	18.55	
ANISOU 893	CE1	TYR	122	2131	2050	2868	102	-404	2 5 1
ATOM 894	CD2	TYR	122	2.445	29.619	51.731	1.000	20.72	
ANISOU 894	CD2	TYR	122	3308	1366	3197	-519	-1524	3 2 3
ATOM 895	CE2	TYR	122	3.140	28.773	52.574	1.000	25.40	
ANISOU 895	CE2	TYR	122	3772	1812	4067	-782	-2084	8 7 3
ATOM 896	CZ	TYR	122	4.413	29.101	52.992	1.000	20.93	
ANISOU 896	CZ	TYR	122	2985	1742	3224	-96	-1145	3 1 3
ATOM 897	OH	TYR	122	5.068	28.230	53.826	1.000	29.87	
ANISOU 897	OH	TYR	122	4830	1998	4522	-680	-3078	6 2 1
ATOM 898	C	TYR	122	3.218	30.876	48.209	1.000	12.33	
ANISOU 898	C	TYR	122	1833	1412	1439	89	-218	8 8
ATOM 899	O	TYR	122	4.395	30.507	48.117	1.000	14.25	
ANISOU 899	O	TYR	122	1896	1861	1656	339	-242	2 1 6
ATOM 900	N	PHE	123	2.224	30.269	47.573	1.000	11.28	
ANISOU 900	N	PHE	123	1950	1297	1041	6	-151	1 8 5
ATOM 901	CA	PHE	123	2.482	29.151	46.665	1.000	12.08	
ANISOU 901	CA	PHE	123	1731	1219	1640	64	-60	2 6
ATOM 902	CB	PHE	123	1.139	28.719	46.024	1.000	13.86	
ANISOU 902	CB	PHE	123	2048	1550	1666	-104	-276	-8 2
ATOM 903	CG	PHE	123	1.311	27.516	45.099	1.000	14.44	
ANISOU 903	CG	PHE	123	2173	1677	1637	142	-475	-9 4
ATOM 904	CD1	PHE	123	1.281	26.234	45.614	1.000	13.64	
ANISOU 904	CD1	PHE	123	1857	1563	1764	-42	-702	-2 3 6
ATOM 905	CD2	PHE	123	1.511	27.664	43.729	1.000	13.81	
ANISOU 905	CD2	PHE	123	1450	2164	1634	-420	-295	-2 4 8
ATOM 906	CE1	PHE	123	1.468	25.141	44.795	1.000	17.16	
ANISOU 906	CE1	PHE	123	2282	1819	2418	130	-855	-6 4 4
ATOM 907	CE2	PHE	123	1.715	26.559	42.916	1.000	18.31	
ANISOU 907	CE2	PHE	123	2098	2657	2201	-1053	172	-8 4 5
ATOM 908	CZ	PHE	123	1.706	25.295	43.445	1.000	16.71	
ANISOU 908	CZ	PHE	123	1442	2382	2526	-36	-306	-1 0 7 7
ATOM 909	C	PHE	123	3.489	29.511	45.581	1.000	13.48	
ANISOU 909	C	PHE	123	2004	1472	1645	236	157	1 8
ATOM 910	O	PHE	123	4.424	28.768	45.242	1.000	13.07	
ANISOU 910	O	PHE	123	1591	1498	1876	42	-78	-1 7 2
ATOM 911	N	ASP	124	3.294	30.684	44.948	1.000	13.83	
ANISOU 911	N	ASP	124	1490	1575	2189	51	207	2 8 8
ATOM 912	CA	ASP	124	4.207	31.036	43.861	1.000	13.75	
ANISOU 912	CA	ASP	124	1505	1330	2389	458	398	3 4 4
ATOM 913	CB	ASP	124	3.708	32.352	43.242	1.000	18.95	
ANISOU 913	CB	ASP	124	2650	1970	2580	656	-63	9 2 6
ATOM 914	CG	ASP	124	4.470	32.708	41.989	1.000	27.54	
ANISOU 914	CG	ASP	124	5327	2099	3036	-123	939	8 8 0
ATOM 915	OD1	ASP	124	4.541	31.904	41.023	1.000	37.04	
ANISOU 915	OD1	ASP	124	6362	3225	4485	108	2616	-3 3 1

- 120 -

ATOM	916	OD2	ASP	124	4.985	33.843	42.011	1.000	32.60
ANISOU	916	OD2	ASP	124	4724	3509	4151	-1539	234 8 5 1
ATOM	917	C	ASP	124	5.645	31.164	44.328	1.000	14.49
ANISOU	917	C	ASP	124	1493	1721	2293	327	485 4 8 2
ATOM	918	O	ASP	124	6.591	30.721	43.674	1.000	14.52
ANISOU	918	O	ASP	124	1477	1363	2679	289	497 3 0 7
ATOM	919	N	ARG	125	5.866	31.777	45.499	1.000	14.03
ANISOU	919	N	ARG	125	1501	1271	2558	353	398 4 1 4
ATOM	920	CA	ARG	125	7.214	31.863	46.044	1.000	16.40
ANISOU	920	CA	ARG	125	1642	1625	2963	194	178 2 2 6
ATOM	921	C	ARG	125	7.828	30.494	46.346	1.000	14.69
ANISOU	921	C	ARG	125	1396	1688	2496	232	-25 1 5 3
ATOM	922	O	ARG	125	8.999	30.245	46.034	1.000	14.10
ANISOU	922	O	ARG	125	1279	1656	2424	7	-205 -2 0 1
ATOM	923	CB	ARG	125	7.213	32.705	47.318	1.000	18.13
ANISOU	923	CB	ARG	125	1950	1902	3035	787	-81 4 6
ATOM	924	CG	ARG	125	7.045	34.193	47.041	1.000	23.51
ANISOU	924	CG	ARG	125	2232	1780	4919	883	-36 -2 2 5
ATOM	925	CD	ARG	125	8.391	34.815	46.694	1.000	29.33
ANISOU	925	CD	ARG	125	3596	2824	4724	-667	237 -1 8 7
ATOM	926	NE	ARG	125	8.194	36.262	46.803	1.000	32.99
ANISOU	926	NE	ARG	125	4350	2766	5418	-678	-1642 1 5 6
ATOM	927	CZ	ARG	125	8.868	37.153	47.495	1.000	27.38
ANISOU	927	CZ	ARG	125	2292	2758	5353	-276	-580 -2 4 6
ATOM	928	NH1	ARG	125	9.916	36.821	48.235	1.000	38.55
ANISOU	928	NH1	ARG	125	4611	3604	6433	449	-2476 -6 6 9
ATOM	929	NH2	ARG	125	8.491	38.423	47.442	1.000	30.26
ANISOU	929	NH2	ARG	125	4062	2570	4865	-369	-835 3 6 3
ATOM	930	N	GLN	126	7.065	29.573	46.920	1.000	12.36
ANISOU	930	N	GLN	126	1316	1376	2002	248	-63 -2 6 4
ATOM	931	CA	GLN	126	7.524	28.201	47.153	1.000	13.39
ANISOU	931	CA	GLN	126	1765	1323	1999	219	-355 -3 7 7
ATOM	932	CB	AGLN	126	6.363	27.455	47.828	0.500	16.24
ANISOU	932	CB	AGLN	126	2422	1391	2357	188	202 -1 9 2
ATOM	933	CG	AGLN	126	6.149	27.758	49.284	0.500	18.83
ANISOU	933	CG	AGLN	126	2761	2021	2371	68	233 -2 1 0
ATOM	934	CD	AGLN	126	7.077	27.146	50.298	0.500	23.94
ANISOU	934	CD	AGLN	126	3578	2745	2774	-604	-757 3 3
ATOM	935	OE1	AGLN	126	7.181	27.683	51.419	0.500	35.94
ANISOU	935	OE1	AGLN	126	6788	3731	3136	-578	-1567 -4 7 8
ATOM	936	NE2	AGLN	126	7.774	26.055	50.008	0.500	24.63
ANISOU	936	NE2	AGLN	126	4491	1118	3751	-881	-2407 4 6 2
ATOM	937	CB	BGLN	126	6.525	27.417	48.018	0.500	13.36
ANISOU	937	CB	BGLN	126	1695	1137	2245	602	-114 -2 5 5
ATOM	938	CG	BGLN	126	6.604	27.750	49.497	0.500	18.28
ANISOU	938	CG	BGLN	126	2537	2257	2153	-68	-176 -1 0 5
ATOM	939	CD	BGLN	126	5.442	27.237	50.319	0.500	18.42
ANISOU	939	CD	BGLN	126	2227	2573	2198	344	-159 1 0 6
ATOM	940	OE1	BGLN	126	5.605	26.442	51.242	0.500	25.36
ANISOU	940	OE1	BGLN	126	3289	3517	2828	-100	-223 9 5 3
ATOM	941	NE2	BGLN	126	4.231	27.685	50.003	0.500	25.02
ANISOU	941	NE2	BGLN	126	2427	2669	4413	1004	-83 -2 9 8
ATOM	942	C	GLN	126	7.860	27.448	45.861	1.000	12.95
ANISOU	942	C	GLN	126	1506	1434	1979	307	-372 -3 6 6
ATOM	943	O	GLN	126	8.859	26.721	45.748	1.000	11.66
ANISOU	943	O	GLN	126	1461	1142	1827	182	-85 1 5 9
ATOM	944	N	TYR	127	6.960	27.578	44.868	1.000	11.61
ANISOU	944	N	TYR	127	1400	1276	1735	146	-168 -1 0
ATOM	945	CA	TYR	127	7.152	26.869	43.585	1.000	11.21
ANISOU	945	CA	TYR	127	1469	1242	1550	-92	-40 1 9 2
ATOM	946	CB	TYR	127	5.901	26.940	42.724	1.000	11.82

- 121 -

ANISOU 946	CB	TYR	127	1346	1655	1491	-13	82	4	7
ATOM 947	CG	TYR	127	5.791	26.069	41.496	1.000	11.	4	9
ANISOU 947	CG	TYR	127	1278	1428	1660	-4	-4	1	0
ATOM 948	CD1	TYR	127	6.550	24.928	41.270	1.000	11.	2	8
ANISOU 948	CD1	TYR	127	1030	1334	1921	-87	-100	3	3
ATOM 949	CE1	TYR	127	6.406	24.153	40.115	1.000	11.	4	7
ANISOU 949	CE1	TYR	127	1164	1167	2027	-51	-53	2	1
ATOM 950	CD2	TYR	127	4.871	26.410	40.500	1.000	11.	9	8
ANISOU 950	CD2	TYR	127	1677	1093	1784	204	-219	-1	0
ATOM 951	CE2	TYR	127	4.715	25.655	39.357	1.000	11.	3	7
ANISOU 951	CE2	TYR	127	1539	1118	1665	140	-68	-7	3
ATOM 952	CZ	TYR	127	5.494	24.508	39.163	1.000	11.	0	2
ANISOU 952	CZ	TYR	127	1202	1226	1760	91	48	-1	2
ATOM 953	OH	TYR	127	5.379	23.720	38.030	1.000	11.	5	7
ANISOU 953	OH	TYR	127	1547	1138	1712	94	177	-3	4
ATOM 954	C	TYR	127	8.386	27.392	42.882	1.000	10.	8	3
ANISOU 954	C	TYR	127	1296	989	1830	230	-43	3	7
ATOM 955	O	TYR	127	9.185	26.605	42.375	1.000	10.	8	6
ANISOU 955	O	TYR	127	1292	1232	1603	164	-237	-4	2
ATOM 956	N	THR	128	8.565	28.716	42.865	1.000	10.	9	8
ANISOU 956	N	THR	128	1554	976	1642	212	-9	5	5
ATOM 957	CA	THR	128	9.766	29.305	42.295	1.000	11.	8	0
ANISOU 957	CA	THR	128	1686	1125	1673	-47	-169	3	8
ATOM 958	CB	THR	128	9.605	30.849	42.378	1.000	12.	6	6
ANISOU 958	CB	THR	128	1873	1074	1864	-52	-233	5	2
ATOM 959	OG1	THR	128	8.530	31.286	41.517	1.000	16.	7	4
ANISOU 959	OG1	THR	128	2223	1597	2542	124	-457	9	9
ATOM 960	CG2	THR	128	10.878	31.510	41.893	1.000	16.	5	4
ANISOU 960	CG2	THR	128	1871	778	3635	262	655	1	3
ATOM 961	C	THR	128	11.040	28.828	42.964	1.000	11.	2	6
ANISOU 961	C	THR	128	1562	980	1738	-71	-162	1	4
ATOM 962	O	THR	128	11.995	28.458	42.258	1.000	12.	1	6
ANISOU 962	O	THR	128	1769	1092	1758	17	26	2	7
ATOM 963	N	ALA	129	11.083	28.802	44.300	1.000	10.	3	9
ANISOU 963	N	ALA	129	1183	1001	1763	70	-118	1	4
ATOM 964	CA	ALA	129	12.273	28.386	45.037	1.000	10.	5	9
ANISOU 964	CA	ALA	129	1206	945	1873	-69	-170	2	8
ATOM 965	CB	ALA	129	12.113	28.603	46.536	1.000	12.	4	6
ANISOU 965	CB	ALA	129	2113	851	1769	82	-218	5	7
ATOM 966	C	ALA	129	12.575	26.906	44.802	1.000	11.	3	5
ANISOU 966	C	ALA	129	1258	883	2170	-16	-141	4	1
ATOM 967	O	ALA	129	13.738	26.485	44.641	1.000	10.	9	3
ANISOU 967	O	ALA	129	1202	1157	1796	-36	-213	1	2
ATOM 968	N	SER	130	11.519	26.086	44.750	1.000	12.	2	7
ANISOU 968	N	SER	130	1280	984	2398	-65	-1	-2	4
ATOM 969	CA	SER	130	11.682	24.650	44.512	1.000	10.	8	9
ANISOU 969	CA	SER	130	1623	876	1638	-85	44	3	7
ATOM 970	CB	ASER	130	10.342	23.940	44.716	0.500	10.	0	8
ANISOU 970	CB	ASER	130	1432	603	1793	213	247	4	1
ATOM 971	OG	ASER	130	9.771	24.063	46.006	0.500	9.	1	2
ANISOU 971	OG	ASER	130	1021	651	1792	91	1	-1	4
ATOM 972	CB	BSER	130	10.364	23.919	44.765	0.500	10.	6	0
ANISOU 972	CB	BSER	130	1687	822	1521	-45	318	1	5
ATOM 973	OG	BSER	130	9.418	24.098	43.734	0.500	16.	2	2
ANISOU 973	OG	BSER	130	1717	1289	3156	137	-525	3	4
ATOM 974	C	SER	130	12.214	24.373	43.110	1.000	10.	5	3
ANISOU 974	C	SER	130	1586	733	1684	-166	210	4	8
ATOM 975	O	SER	130	13.137	23.532	42.942	1.000	11.	1	7
ANISOU 975	O	SER	130	1385	1012	1849	-151	-95	1	4
ATOM 976	N	ARG	131	11.680	25.044	42.079	1.000	10.	4	6
ANISOU 976	N	ARG	131	1578	861	1534	-87	-66	9	9

- 122 -

ATOM	977	CA	ARG	131	12.260	24.839	40.742	1.000	10.60
ANISOU	977	CA	ARG	131	1480	1110	1438	61	-288 8 2
ATOM	978	CB	ARG	131	11.426	25.553	39.679	1.000	12.99
ANISOU	978	CB	ARG	131	1893	1369	1673	63	-525 2 7 6
ATOM	979	CG	ARG	131	10.003	25.065	39.431	1.000	13.64
ANISOU	979	CG	ARG	131	1707	1735	1742	335	-559 - 8 6
ATOM	980	CD	ARG	131	9.349	25.669	38.206	1.000	17.71
ANISOU	980	CD	ARG	131	2078	1973	2677	81	-983 7 0 1
ATOM	981	NE	ARG	131	9.453	27.113	38.015	1.000	19.76
ANISOU	981	NE	ARG	131	2716	2034	2757	-25	-525 7 1 3
ATOM	982	CZ	ARG	131	8.629	28.004	38.568	1.000	21.24
ANISOU	982	CZ	ARG	131	3688	1878	2503	-8	-128 6 4 7
ATOM	983	NH1	ARG	131	7.631	27.634	39.366	1.000	21.32
ANISOU	983	NH1	ARG	131	2792	3142	2166	-486	-667 5 7
ATOM	984	NH2	ARG	131	8.771	29.310	38.361	1.000	27.83
ANISOU	984	NH2	ARG	131	4649	1822	4103	-90	-422 5 6 1
ATOM	985	C	ARG	131	13.714	25.323	40.688	1.000	10.42
ANISOU	985	C	ARG	131	1542	1078	1339	50	-103 1
ATOM	986	O	ARG	131	14.568	24.683	40.080	1.000	10.94
ANISOU	986	O	ARG	131	1544	1105	1506	177	-134 4 2
ATOM	987	N	ALA	132	14.028	26.438	41.343	1.000	10.97
ANISOU	987	N	ALA	132	1477	1129	1563	74	-364 - 4 5
ATOM	988	CA	ALA	132	15.379	26.983	41.343	1.000	11.10
ANISOU	988	CA	ALA	132	1539	944	1735	9	-102 9 7
ATOM	989	CB	ALA	132	15.429	28.344	42.048	1.000	12.82
ANISOU	989	CB	ALA	132	1711	1171	1987	-48	-248 - 1 9 8
ATOM	990	C	ALA	132	16.393	26.045	41.995	1.000	11.55
ANISOU	990	C	ALA	132	1085	1107	2197	-197	305 7 4 5
ATOM	991	O	ALA	132	17.481	25.832	41.432	1.000	11.81
ANISOU	991	O	ALA	132	1081	1809	1599	-204	17 - 9
ATOM	992	N	VAL	133	16.061	25.490	43.175	1.000	11.16
ANISOU	992	N	VAL	133	1260	1356	1623	-148	51 3 5 0
ATOM	993	CA	VAL	133	17.011	24.587	43.840	1.000	11.62
ANISOU	993	CA	VAL	133	1505	1529	1380	-69	-297 8 9
ATOM	994	CB	VAL	133	16.738	24.418	45.344	1.000	12.14
ANISOU	994	CB	VAL	133	1376	1674	1564	-74	-25 3 6 4
ATOM	995	CG1	VAL	133	15.550	23.501	45.608	1.000	14.96
ANISOU	995	CG1	VAL	133	1705	2316	1662	-706	8 - 3 5 7
ATOM	996	CG2	VAL	133	17.981	23.864	46.033	1.000	15.63
ANISOU	996	CG2	VAL	133	1755	2340	1845	-341	-677 5 5 1
ATOM	997	C	VAL	133	17.079	23.268	43.065	1.000	11.71
ANISOU	997	C	VAL	133	1376	1363	1711	-24	-425 1 6 9
ATOM	998	O	VAL	133	18.198	22.733	42.925	1.000	11.55
ANISOU	998	O	VAL	133	1391	1453	1545	-4	-116 3 9 8
ATOM	999	N	ALA	134	15.982	22.758	42.480	1.000	12.87
ANISOU	999	N	ALA	134	1399	1517	1973	28	-334 - 2 2 8
ATOM	1000	CA	ALA	134	16.084	21.557	41.621	1.000	10.57
ANISOU	1000	CA	ALA	134	1106	1220	1691	153	-298 9 6
ATOM	1001	CB	ALA	134	14.699	21.096	41.186	1.000	12.20
ANISOU	1001	CB	ALA	134	1254	1589	1794	35	-303 - 1 2 7
ATOM	1002	C	ALA	134	16.968	21.797	40.399	1.000	12.58
ANISOU	1002	C	ALA	134	1393	1399	1987	272	-4 2 7 7
ATOM	1003	O	ALA	134	17.712	20.924	39.970	1.000	11.01
ANISOU	1003	O	ALA	134	1254	1358	1574	83	-268 2 6
ATOM	1004	N	ARG	135	16.908	22.995	39.809	1.000	12.03
ANISOU	1004	N	ARG	135	1517	1230	1824	-62	-327 8 7
ATOM	1005	CA	ARG	135	17.773	23.353	38.676	1.000	13.23
ANISOU	1005	CA	ARG	135	1854	1158	2015	-270	-209 1 6 1
ATOM	1006	CB	ARG	135	17.393	24.734	38.170	1.000	14.57
ANISOU	1006	CB	ARG	135	2203	1339	1994	-45	-541 2 2 2
ATOM	1007	CG	ARG	135	17.753	25.160	36.797	1.000	19.22

- 123 -

ANISOU	1007	CG	ARG	135	4204	1120	1980	-490	-433	1 5 0
ATOM	1008	CD	ARG	135	17.237	26.563	36.471	1.000	22.14	
ANISOU	1008	CD	ARG	135	4046	1500	2868	-159	315	8 2 2
ATOM	1009	NE	ARG	135	15.831	26.607	36.077	1.000	22.66	
ANISOU	1009	NE	ARG	135	4239	1404	2965	-94	47	2 5 7
ATOM	1010	CZ	ARG	135	14.802	27.184	36.684	1.000	21.69	
ANISOU	1010	CZ	ARG	135	4004	1906	2333	92	-506	6 4
ATOM	1011	NH1	ARG	135	14.917	27.843	37.833	1.000	22.26	
ANISOU	1011	NH1	ARG	135	4114	2532	1812	460	-833	3 4 1
ATOM	1012	NH2	ARG	135	13.582	27.113	36.149	1.000	22.31	
ANISOU	1012	NH2	ARG	135	4000	2243	2234	-544	-419	8
ATOM	1013	C	ARG	135	19.251	23.275	39.057	1.000	12.70	
ANISOU	1013	C	ARG	135	1742	1264	1821	-119	-16	4 3 0
ATOM	1014	O	ARG	135	20.069	22.818	38.238	1.000	14.67	
ANISOU	1014	O	ARG	135	2133	1529	1910	19	169	3 9 1
ATOM	1015	N	GLU	136	19.572	23.712	40.266	1.000	12.15	
ANISOU	1015	N	GLU	136	1423	1372	1820	-36	70	4 3 0
ATOM	1016	CA	GLU	136	20.960	23.630	40.763	1.000	14.52	
ANISOU	1016	CA	GLU	136	1622	1701	2194	-90	-197	3 7 1
ATOM	1017	CB	GLU	136	21.212	24.513	41.981	1.000	15.59	
ANISOU	1017	CB	GLU	136	1502	1781	2642	14	-231	1 1
ATOM	1018	CG	GLU	136	21.064	26.020	41.783	1.000	18.01	
ANISOU	1018	CG	GLU	136	2010	1762	3071	-232	-153	1 2 6
ATOM	1019	CD	GLU	136	21.798	26.484	40.537	1.000	20.18	
ANISOU	1019	CD	GLU	136	2071	2079	3519	-308	89	3 6 9
ATOM	1020	OE1	GLU	136	22.987	26.148	40.394	1.000	24.64	
ANISOU	1020	OE1	GLU	136	2060	2937	4364	-262	338	6 1 5
ATOM	1021	OE2	GLU	136	21.195	27.150	39.670	1.000	24.19	
ANISOU	1021	OE2	GLU	136	2479	2327	4385	-381	317	1 4 2 6
ATOM	1022	C	GLU	136	21.364	22.186	41.076	1.000	14.00	
ANISOU	1022	C	GLU	136	1338	1619	2361	-112	-442	2 2 3
ATOM	1023	O	GLU	136	22.508	21.781	40.833	1.000	13.86	
ANISOU	1023	O	GLU	136	1366	1890	2009	-100	-287	3 2 9
ATOM	1024	N	VAL	137	20.472	21.338	41.580	1.000	11.78	
ANISOU	1024	N	VAL	137	1309	1451	1715	148	-223	8 5
ATOM	1025	CA	VAL	137	20.753	19.896	41.771	1.000	12.49	
ANISOU	1025	CA	VAL	137	1369	1522	1853	240	-69	2 8 9
ATOM	1026	CB	VAL	137	19.560	19.165	42.429	1.000	12.41	
ANISOU	1026	CB	VAL	137	1422	1424	1869	-67	-85	- 2 0 4
ATOM	1027	CG1	VAL	137	19.728	17.634	42.401	1.000	12.55	
ANISOU	1027	CG1	VAL	137	1371	1508	1892	182	185	1 1 1
ATOM	1028	CG2	VAL	137	19.355	19.607	43.852	1.000	11.35	
ANISOU	1028	CG2	VAL	137	1461	1281	1572	182	-254	2 8 8
ATOM	1029	C	VAL	137	21.100	19.241	40.435	1.000	12.48	
ANISOU	1029	C	VAL	137	1202	1428	2113	150	-16	8 5
ATOM	1030	O	VAL	137	22.057	18.462	40.287	1.000	13.03	
ANISOU	1030	O	VAL	137	1021	1683	2249	149	1	1 4 6
ATOM	1031	N	LEU	138	20.309	19.562	39.401	1.000	10.28	
ANISOU	1031	N	LEU	138	1198	881	1829	-15	158	2 2 6
ATOM	1032	CA	LEU	138	20.571	19.029	38.066	1.000	12.48	
ANISOU	1032	CA	LEU	138	1312	1408	2024	110	273	- 5 2
ATOM	1033	CB	LEU	138	19.398	19.358	37.130	1.000	11.81	
ANISOU	1033	CB	LEU	138	1260	1586	1642	-20	383	4 3
ATOM	1034	CG	LEU	138	18.036	18.726	37.457	1.000	10.77	
ANISOU	1034	CG	LEU	138	1391	1397	1304	-83	219	2 1 3
ATOM	1035	CD1	LEU	138	16.916	19.324	36.596	1.000	12.72	
ANISOU	1035	CD1	LEU	138	1416	1587	1829	-59	-25	1 7 3
ATOM	1036	CD2	LEU	138	18.052	17.207	37.320	1.000	14.32	
ANISOU	1036	CD2	LEU	138	1986	1390	2065	-79	296	3 7 0
ATOM	1037	C	LEU	138	21.903	19.525	37.505	1.000	13.61	
ANISOU	1037	C	LEU	138	1305	2026	1840	-65	174	5

- 124 -

ATOM 1038 O LEU 138 22.695 18.760 36.920 1.000 14.97
 ANISOU 1038 O LEU 138 1125 2247 2313 105 234 1 7 8
 ATOM 1039 N ARG 139 22.184 20.816 37.614 1.000 13.26
 ANISOU 1039 N ARG 139 1432 2046 1561 -155 219 3 1 7
 ATOM 1040 CA ARG 139 23.397 21.372 37.085 1.000 14.71
 ANISOU 1040 CA ARG 139 1648 1941 2000 -27 502 4 4 7
 ATOM 1041 C ARG 139 24.636 20.815 37.775 1.000 15.16
 ANISOU 1041 C ARG 139 1425 2101 2235 -158 324 1 1 6
 ATOM 1042 O ARG 139 25.650 20.495 37.166 1.000 18.15
 ANISOU 1042 O ARG 139 1628 2581 2688 18 612 3 3 9
 ATOM 1043 CB ARG 139 23.394 22.926 37.206 1.000 19.67
 ANISOU 1043 CB ARG 139 1749 1923 3803 -196 186 2 5 2
 ATOM 1044 CG ARG 139 24.418 23.487 36.237 1.000 28.66
 ANISOU 1044 CG ARG 139 3924 2584 4383 -2305 882 -5 6 3
 ATOM 1045 CD ARG 139 24.245 24.997 36.111 1.000 39.58
 ANISOU 1045 CD ARG 139 6801 2389 5849 -3273 119 -3 0 6
 ATOM 1046 NE ARG 139 24.910 25.660 37.210 1.000 47.91
 ANISOU 1046 NE ARG 139 9548 2435 6222 -2157 -1331 -7 0 8
 ATOM 1047 CZ ARG 139 24.493 26.682 37.928 1.000 45.42
 ANISOU 1047 CZ ARG 139 6941 4516 5802 -882 -2118 -12 3 8
 ATOM 1048 NH1 ARG 139 23.316 27.273 37.722 1.000 64.33
 ANISOU 1048 NH1 ARG 139 7248 8153 9039 93 -2965 -9 8 0
 ATOM 1049 NH2 ARG 139 25.309 27.109 38.888 1.000 32.62
 ANISOU 1049 NH2 ARG 139 5020 4758 2616 -2746 590 1 6 7
 ATOM 1050 N ALA 140 24.562 20.684 39.096 1.000 14.85
 ANISOU 1050 N ALA 140 1287 2204 2151 -517 -26 -4 6
 ATOM 1051 CA ALA 140 25.730 20.257 39.856 1.000 15.80
 ANISOU 1051 CA ALA 140 989 2649 2366 -309 -9 -4 0 1
 ATOM 1052 CB ALA 140 25.444 20.442 41.330 1.000 19.36
 ANISOU 1052 CB ALA 140 2685 2447 2222 243 -435 -4 8 0
 ATOM 1053 C ALA 140 26.111 18.806 39.584 1.000 16.86
 ANISOU 1053 C ALA 140 1555 2795 2054 12 -186 -4 5 8
 ATOM 1054 O ALA 140 27.258 18.403 39.796 1.000 18.90
 ANISOU 1054 O ALA 140 1538 2686 2958 -21 60 1 4 5
 ATOM 1055 N THR 141 25.147 18.025 39.098 1.000 17.53
 ANISOU 1055 N THR 141 1779 2532 2350 -528 218 -1 0 8
 ATOM 1056 CA THR 141 25.340 16.625 38.765 1.000 15.59
 ANISOU 1056 CA THR 141 1256 2401 2268 -192 -95 2 9 1
 ATOM 1057 CB THR 141 24.207 15.735 39.343 1.000 14.77
 ANISOU 1057 CB THR 141 1238 2200 2172 155 282 3 0 1
 ATOM 1058 OG1 THR 141 22.946 16.168 38.849 1.000 12.47
 ANISOU 1058 OG1 THR 141 1249 1565 1926 -31 295 4 7 6
 ATOM 1059 CG2 THR 141 24.167 15.818 40.859 1.000 14.82
 ANISOU 1059 CG2 THR 141 1394 2077 2160 135 -47 1 7 7
 ATOM 1060 C THR 141 25.423 16.374 37.257 1.000 16.11
 ANISOU 1060 C THR 141 1732 2046 2343 303 583 3 2 5
 ATOM 1061 O THR 141 25.432 15.235 36.778 1.000 17.55
 ANISOU 1061 O THR 141 1991 2104 2573 237 555 2 4 9
 ATOM 1062 N GLY 142 25.474 17.416 36.446 1.000 17.74
 ANISOU 1062 N GLY 142 2127 2197 2416 303 260 5 0 1
 ATOM 1063 CA GLY 142 25.611 17.263 34.987 1.000 17.32
 ANISOU 1063 CA GLY 142 1642 2494 2447 -160 453 5 1 7
 ATOM 1064 C GLY 142 24.426 16.556 34.358 1.000 16.37
 ANISOU 1064 C GLY 142 1619 1893 2710 261 472 4 2
 ATOM 1065 O GLY 142 24.654 15.824 33.379 1.000 18.43
 ANISOU 1065 O GLY 142 2243 2558 2201 57 798 1 6 3
 ATOM 1066 N THR 143 23.232 16.738 34.907 1.000 13.99
 ANISOU 1066 N THR 143 1531 1429 2356 83 430 3 5 0
 ATOM 1067 CA THR 143 22.049 16.003 34.472 1.000 14.69
 ANISOU 1067 CA THR 143 1768 1591 2223 8 342 9 3
 ATOM 1068 CB THR 143 21.208 15.584 35.700 1.000 15.52

- 125 -

ANISOU	1068	CB	THR	143	1457	1653	2785	55	419	5	2	9	
ATOM	1069	OG1	THR	143	22.037	14.784	36.573	1.000	14	.	6	3	
ANISOU	1069	OG1	THR	143	1296	1792	2471	52	434	3	6	9	
ATOM	1070	CG2	THR	143	20.044	14.738	35.231	1.000	14	.	2	4	
ANISOU	1070	CG2	THR	143	1761	1981	1669	3	379	1	9	2	
ATOM	1071	C	THR	143	21.135	16.785	33.532	1.000	13	.	9	6	
ANISOU	1071	C	THR	143	1553	1708	2044	128	479	-	1	3	1
ATOM	1072	O	THR	143	20.642	17.828	33.923	1.000	15	.	6	5	
ANISOU	1072	O	THR	143	2374	1580	1995	315	486	5	5		
ATOM	1073	N	GLU	144	20.928	16.279	32.322	1.000	15	.	3	2	
ANISOU	1073	N	GLU	144	1734	1904	2184	-156	260	-	2	7	1
ATOM	1074	CA	GLU	144	19.917	16.693	31.362	1.000	17	.	3	0	
ANISOU	1074	CA	GLU	144	1686	2470	2417	-377	152	1	0	6	
ATOM	1075	C	GLU	144	18.774	15.693	31.292	1.000	16	.	8	4	
ANISOU	1075	C	GLU	144	1633	2380	2386	-298	313	-	2	4	2
ATOM	1076	O	GLU	144	18.922	14.631	30.680	1.000	16	.	7	1	
ANISOU	1076	O	GLU	144	1470	2057	2821	-43	610	5	8		
ATOM	1077	CB	GLU	144	20.539	16.856	29.970	1.000	21	.	9	1	
ANISOU	1077	CB	GLU	144	2747	3417	2162	-1508	31	-	8		
ATOM	1078	CG	GLU	144	19.568	17.063	28.825	1.000	37	.	9	3	
ANISOU	1078	CG	GLU	144	6652	4374	3385	-2057	-2082	1	7	6	7
ATOM	1079	CD	GLU	144	19.293	18.507	28.466	1.000	43	.	5	5	
ANISOU	1079	CD	GLU	144	7869	4258	4419	-2497	-2259	2	1	2	9
ATOM	1080	OE1	GLU	144	19.602	19.365	29.326	1.000	51	.	8	1	
ANISOU	1080	OE1	GLU	144	9843	4613	5230	-3180	-832	1	1	2	6
ATOM	1081	OE2	GLU	144	18.766	18.798	27.367	1.000	40	.	1	2	
ANISOU	1081	OE2	GLU	144	5551	6029	3662	-285	-115	2	6	6	0
ATOM	1082	N	PRO	145	17.620	15.959	31.908	1.000	14	.	2	9	
ANISOU	1082	N	PRO	145	1634	1364	2432	-4	208	2	6	5	
ATOM	1083	CD	PRO	145	17.256	17.136	32.718	1.000	14	.	1	4	
ANISOU	1083	CD	PRO	145	1735	1778	1859	-55	32	1	6	7	
ATOM	1084	CA	PRO	145	16.507	15.000	31.807	1.000	13	.	7	2	
ANISOU	1084	CA	PRO	145	1484	1391	2337	66	173	4	6	6	
ATOM	1085	CB	PRO	145	15.406	15.701	32.606	1.000	14	.	2	0	
ANISOU	1085	CB	PRO	145	1459	1636	2302	161	-41	2	8	9	
ATOM	1086	CG	PRO	145	16.132	16.608	33.561	1.000	14	.	4	3	
ANISOU	1086	CG	PRO	145	1796	2007	1679	-23	-42	4	4	9	
ATOM	1087	C	PRO	145	16.076	14.794	30.372	1.000	15	.	1	8	
ANISOU	1087	C	PRO	145	1745	1665	2359	-192	231	2	8	7	
ATOM	1088	O	PRO	145	16.178	15.685	29.509	1.000	15	.	4	0	
ANISOU	1088	O	PRO	145	2430	1511	1910	-85	613	-	1	5	
ATOM	1089	N	ASP	146	15.544	13.613	30.070	1.000	15	.	7	9	
ANISOU	1089	N	ASP	146	2019	1611	2367	-191	666	8	1		
ATOM	1090	CA	ASP	146	14.918	13.366	28.773	1.000	16	.	7	4	
ANISOU	1090	CA	ASP	146	2095	1759	2506	-348	575	-	7	7	
ATOM	1091	CB	ASP	146	14.300	11.966	28.727	1.000	18	.	9	9	
ANISOU	1091	CB	ASP	146	2508	1729	2977	-323	780	-	4	3	9
ATOM	1092	CG	ASP	146	13.504	11.784	27.444	1.000	27	.	0	4	
ANISOU	1092	CG	ASP	146	4012	2450	3813	-720	-229	-	8	0	5
ATOM	1093	OD1	ASP	146	12.295	12.121	27.409	1.000	38	.	6	5	
ANISOU	1093	OD1	ASP	146	3943	4889	5852	-595	-1282	-	3	2	3
ATOM	1094	OD2	ASP	146	14.091	11.311	26.466	1.000	39	.	9	5	
ANISOU	1094	OD2	ASP	146	6913	5052	3214	16	0	-	1	1	8
ATOM	1095	C	ASP	146	13.860	14.441	28.552	1.000	16	.	6	5	
ANISOU	1095	C	ASP	146	2461	1904	1961	-128	580	-	4	0	
ATOM	1096	O	ASP	146	13.041	14.605	29.457	1.000	15	.	6	7	
ANISOU	1096	O	ASP	146	2110	1935	1908	-334	381	-	4	2	0
ATOM	1097	N	GLY	147	13.871	15.149	27.429	1.000	20	.	6	0	
ANISOU	1097	N	GLY	147	3484	2416	1927	-26	419	1	2	9	
ATOM	1098	CA	GLY	147	12.903	16.212	27.155	1.000	18	.	0	6	
ANISOU	1098	CA	GLY	147	2771	2451	1638	-382	98	9	3		

- 126 -

ATOM 1099 C GLY 147 13.361 17.574 27.609 1.000 18.73
 ANISOU 1099 C GLY 147 2836 2195 2085 -524 143 5 2 7
 ATOM 1100 O GLY 147 12.676 18.570 27.282 1.000 18.34
 ANISOU 1100 O GLY 147 2865 2416 1687 -413 -72 3 8 9
 ATOM 1101 N GLY 148 14.498 17.634 28.316 1.000 16.35
 ANISOU 1101 N GLY 148 2936 1506 1772 -157 142 8 8
 ATOM 1102 CA GLY 148 15.116 18.889 28.747 1.000 15.34
 ANISOU 1102 CA GLY 148 2723 1279 1829 55 450 - 2 6
 ATOM 1103 C GLY 148 14.768 19.339 30.144 1.000 12.97
 ANISOU 1103 C GLY 148 2231 1416 1280 -93 -62 4 0 7
 ATOM 1104 O GLY 148 13.769 18.930 30.771 1.000 13.79
 ANISOU 1104 O GLY 148 2301 1376 1561 -164 88 3 2 3
 ATOM 1105 N VAL 149 15.604 20.224 30.718 1.000 12.81
 ANISOU 1105 N VAL 149 1815 1366 1686 155 -31 2 3 8
 ATOM 1106 CA VAL 149 15.388 20.724 32.079 1.000 11.81
 ANISOU 1106 CA VAL 149 1333 1390 1765 54 -92 1 2 9
 ATOM 1107 CB VAL 149 16.594 21.636 32.480 1.000 11.97
 ANISOU 1107 CB VAL 149 1136 1696 1717 -100 246 1 2 4
 ATOM 1108 CG1 VAL 149 16.358 22.336 33.802 1.000 15.26
 ANISOU 1108 CG1 VAL 149 1941 1922 1936 -195 55 - 2 2 3
 ATOM 1109 CG2 VAL 149 17.868 20.794 32.538 1.000 17.21
 ANISOU 1109 CG2 VAL 149 1231 2045 3265 45 102 - 1 0 3
 ATOM 1110 C VAL 149 14.101 21.482 32.280 1.000 11.32
 ANISOU 1110 C VAL 149 1186 1303 1813 -78 131 4 7 9
 ATOM 1111 O VAL 149 13.378 21.218 33.253 1.000 12.35
 ANISOU 1111 O VAL 149 1664 1423 1608 -71 229 1 6 7
 ATOM 1112 N GLU 150 13.752 22.463 31.460 1.000 11.96
 ANISOU 1112 N GLU 150 1347 1453 1746 29 -36 4 2 0
 ATOM 1113 CA GLU 150 12.592 23.286 31.815 1.000 10.90
 ANISOU 1113 CA GLU 150 1623 1359 1159 118 0 4 0 5
 ATOM 1114 CB GLU 150 12.608 24.601 30.999 1.000 17.60
 ANISOU 1114 CB GLU 150 2530 1470 2687 181 -161 9 0 7
 ATOM 1115 CG GLU 150 13.811 25.488 31.314 1.000 17.86
 ANISOU 1115 CG GLU 150 2744 797 3246 246 434 2 0 2
 ATOM 1116 CD GLU 150 13.956 25.929 32.738 1.000 19.47
 ANISOU 1116 CD GLU 150 3018 1353 3027 -97 -84 6 6 2
 ATOM 1117 OE1 GLU 150 12.951 26.005 33.475 1.000 18.21
 ANISOU 1117 OE1 GLU 150 3035 1512 2373 -178 -321 5 3 6
 ATOM 1118 OE2 GLU 150 15.109 26.237 33.122 1.000 22.59
 ANISOU 1118 OE2 GLU 150 2993 1664 3927 -38 -150 2 8 4
 ATOM 1119 C GLU 150 11.277 22.533 31.705 1.000 12.22
 ANISOU 1119 C GLU 150 1429 1540 1676 235 147 - 5
 ATOM 1120 O GLU 150 10.341 22.757 32.530 1.000 13.44
 ANISOU 1120 O GLU 150 1739 1474 1894 315 470 2 8 8
 ATOM 1121 N ALA 151 11.118 21.625 30.742 1.000 11.88
 ANISOU 1121 N ALA 151 1783 1255 1477 94 45 2 5 3
 ATOM 1122 CA ALA 151 9.881 20.844 30.698 1.000 13.82
 ANISOU 1122 CA ALA 151 1744 2054 1454 -100 -413 3 9 6
 ATOM 1123 CB ALA 151 9.739 20.094 29.390 1.000 14.89
 ANISOU 1123 CB ALA 151 1489 2318 1851 22 -269 - 3 5
 ATOM 1124 C ALA 151 9.792 19.864 31.867 1.000 12.71
 ANISOU 1124 C ALA 151 1448 1463 1920 93 41 4 2 4
 ATOM 1125 O ALA 151 8.655 19.580 32.280 1.000 14.69
 ANISOU 1125 O ALA 151 1535 2114 1932 -242 204 - 1 0 8
 ATOM 1126 N PHE 152 10.925 19.401 32.410 1.000 11.73
 ANISOU 1126 N PHE 152 1598 1259 1598 120 9 2 7 1
 ATOM 1127 CA PHE 152 10.890 18.554 33.602 1.000 10.61
 ANISOU 1127 CA PHE 152 1444 1061 1526 -33 34 1 6 0
 ATOM 1128 CB PHE 152 12.293 17.981 33.820 1.000 10.23
 ANISOU 1128 CB PHE 152 1317 1132 1437 -144 207 4 1 0
 ATOM 1129 CG PHE 152 12.517 17.187 35.095 1.000 10.36

- 127 -

ANISOU 1129 CG PHE 152 1388 1149 1399 -34 147 2 7 6
 ATOM 1130 CD1 PHE 152 12.036 15.896 35.229 1.000 11.24
 ANISOU 1130 CD1 PHE 152 1479 1047 1743 114 -103 5 6 6
 ATOM 1131 CD2 PHE 152 13.229 17.701 36.154 1.000 11.21
 ANISOU 1131 CD2 PHE 152 1489 1449 1319 85 174 1 5 1
 ATOM 1132 CE1 PHE 152 12.252 15.163 36.380 1.000 10.80
 ANISOU 1132 CE1 PHE 152 1400 1234 1467 249 -111 3 7 3
 ATOM 1133 CE2 PHE 152 13.431 16.992 37.341 1.000 11.82
 ANISOU 1133 CE2 PHE 152 1709 1622 1160 -276 414 2 5 0
 ATOM 1134 CZ PHE 152 12.932 15.717 37.457 1.000 11.97
 ANISOU 1134 CZ PHE 152 1651 1604 1293 -255 296 1 7 0
 ATOM 1135 C PHE 152 10.430 19.292 34.858 1.000 12.24
 ANISOU 1135 C PHE 152 1754 1168 1730 -10 339 8 4
 ATOM 1136 O PHE 152 9.728 18.729 35.726 1.000 11.49
 ANISOU 1136 O PHE 152 1672 1142 1550 200 109 2 7 7
 ATOM 1137 N LEU 153 10.809 20.575 34.997 1.000 11.86
 ANISOU 1137 N LEU 153 2030 1236 1240 -6 73 1 5 6
 ATOM 1138 CA LEU 153 10.532 21.386 36.155 1.000 11.99
 ANISOU 1138 CA LEU 153 1890 1229 1437 -165 307 8 5
 ATOM 1139 CB LEU 153 11.654 22.420 36.353 1.000 12.81
 ANISOU 1139 CB LEU 153 1691 1381 1794 -72 97 -4 0
 ATOM 1140 CG LEU 153 13.059 21.910 36.592 1.000 12.87
 ANISOU 1140 CG LEU 153 1762 1645 1483 146 269 6 4
 ATOM 1141 CD1 LEU 153 14.027 23.081 36.611 1.000 15.99
 ANISOU 1141 CD1 LEU 153 1609 2006 2462 -49 450 -4 3 1
 ATOM 1142 CD2 LEU 153 13.185 21.158 37.914 1.000 19.37
 ANISOU 1142 CD2 LEU 153 3091 2462 1806 809 275 5 4 0
 ATOM 1143 C LEU 153 9.179 22.084 36.123 1.000 12.96
 ANISOU 1143 C LEU 153 1728 1253 1943 -336 360 -4 3
 ATOM 1144 O LEU 153 8.709 22.506 37.193 1.000 13.24
 ANISOU 1144 O LEU 153 1617 1302 2109 -443 481 -1 8 2
 ATOM 1145 N ASP 154 8.568 22.203 34.955 1.000 13.29
 ANISOU 1145 N ASP 154 1643 1457 1951 60 517 2 8 0
 ATOM 1146 CA ASP 154 7.195 22.671 34.764 1.000 14.21
 ANISOU 1146 CA ASP 154 1862 1255 2280 313 631 6 8 3
 ATOM 1147 CB ASP 154 6.995 23.269 33.373 1.000 18.38
 ANISOU 1147 CB ASP 154 2091 2156 2738 328 728 1 4 7 5
 ATOM 1148 CG ASP 154 5.534 23.367 32.929 1.000 22.95
 ANISOU 1148 CG ASP 154 2323 3543 2855 676 430 1 5 0 1
 ATOM 1149 OD1 ASP 154 4.685 23.607 33.820 1.000 20.85
 ANISOU 1149 OD1 ASP 154 2164 2368 3389 895 478 1 1 4 4
 ATOM 1150 OD2 ASP 154 5.168 23.254 31.702 1.000 24.33
 ANISOU 1150 OD2 ASP 154 2989 3146 3110 228 48 1 1 2 8
 ATOM 1151 C ASP 154 6.294 21.455 34.985 1.000 11.22
 ANISOU 1151 C ASP 154 1594 1403 1265 123 147 4 1 0
 ATOM 1152 O ASP 154 6.043 20.729 34.015 1.000 13.31
 ANISOU 1152 O ASP 154 2143 1728 1186 427 219 1 7 0
 ATOM 1153 N CYS 155 5.891 21.220 36.233 1.000 9.91
 ANISOU 1153 N CYS 155 1425 1098 1243 -76 186 2 7
 ATOM 1154 CA CYS 155 5.446 19.881 36.627 1.000 9.41
 ANISOU 1154 CA CYS 155 1294 1168 1115 -13 154 1 7 2
 ATOM 1155 CB CYS 155 6.635 19.171 37.269 1.000 10.64
 ANISOU 1155 CB CYS 155 1276 1015 1753 28 -51 -1 2 2
 ATOM 1156 SG CYS 155 7.316 19.819 38.797 1.000 12.01
 ANISOU 1156 SG CYS 155 1376 1554 1633 -195 -199 9 5
 ATOM 1157 C CYS 155 4.138 19.885 37.423 1.000 9.66
 ANISOU 1157 C CYS 155 1301 1355 1013 115 146 2 1 6
 ATOM 1158 O CYS 155 3.215 20.645 37.064 1.000 11.61
 ANISOU 1158 O CYS 155 1349 1386 1676 130 116 2 9 4
 ATOM 1159 N GLU 156 4.021 19.033 38.442 1.000 10.26
 ANISOU 1159 N GLU 156 1263 1495 1139 -29 168 2 9 9

- 128 -

ATOM 1160 CA GLU 156 2.778 18.787 39.173 1.000 9.04
 ANISOU 1160 CA GLU 156 998 1160 1278 -76 -37 2 3 6
 ATOM 1161 CB GLU 156 2.300 17.391 38.772 1.000 11.63
 ANISOU 1161 CB GLU 156 1187 1348 1885 -67 -135 -190
 ATOM 1162 CG GLU 156 1.841 17.282 37.326 1.000 14.29
 ANISOU 1162 CG GLU 156 1741 1640 2049 -628 -507 5 0
 ATOM 1163 CD GLU 156 0.502 17.949 37.039 1.000 17.90
 ANISOU 1163 CD GLU 156 1772 2692 2336 -365 -686 1 3 7
 ATOM 1164 OE1 GLU 156 -0.220 18.241 38.024 1.000 19.17
 ANISOU 1164 OE1 GLU 156 1429 2973 2884 -632 -270 2 5 3
 ATOM 1165 OE2 GLU 156 0.136 18.198 35.858 1.000 22.03
 ANISOU 1165 OE2 GLU 156 2449 3269 2653 -243 -721 9 2 4
 ATOM 1166 C GLU 156 2.961 18.942 40.677 1.000 9.21
 ANISOU 1166 C GLU 156 1166 1135 1197 -26 239 1 8 3
 ATOM 1167 O GLU 156 2.828 17.997 41.476 1.000 11.22
 ANISOU 1167 O GLU 156 1631 1199 1434 103 162 4 3 1
 ATOM 1168 N PRO 157 3.337 20.158 41.118 1.000 10.29
 ANISOU 1168 N PRO 157 1329 1201 1381 -109 21 1 2 3
 ATOM 1169 CD PRO 157 3.527 21.407 40.359 1.000 10.17
 ANISOU 1169 CD PRO 157 1381 1093 1391 -40 -30 2 1
 ATOM 1170 CA PRO 157 3.618 20.363 42.553 1.000 10.28
 ANISOU 1170 CA PRO 157 1160 1354 1391 -12 -61 6 4
 ATOM 1171 CB PRO 157 4.173 21.805 42.590 1.000 12.44
 ANISOU 1171 CB PRO 157 1832 1567 1330 -397 20 5 8
 ATOM 1172 CG PRO 157 3.475 22.471 41.429 1.000 10.44
 ANISOU 1172 CG PRO 157 1469 1259 1237 -388 166 -1 5
 ATOM 1173 C PRO 157 2.387 20.269 43.450 1.000 10.83
 ANISOU 1173 C PRO 157 1206 1554 1357 -89 -61 7 6
 ATOM 1174 O PRO 157 1.247 20.422 42.992 1.000 11.38
 ANISOU 1174 O PRO 157 1157 1742 1426 -93 -64 3 3
 ATOM 1175 N LEU 158 2.561 19.988 44.742 1.000 9.91
 ANISOU 1175 N LEU 158 1011 1308 1447 -86 -53 1 5 1
 ATOM 1176 CA LEU 158 1.524 19.940 45.764 1.000 10.85
 ANISOU 1176 CA LEU 158 1319 1461 1344 -387 -2 -3
 ATOM 1177 CB LEU 158 1.152 18.482 46.078 1.000 11.03
 ANISOU 1177 CB LEU 158 1280 1447 1464 -251 99 9 3
 ATOM 1178 CG LEU 158 0.111 18.239 47.155 1.000 12.01
 ANISOU 1178 CG LEU 158 1271 1497 1795 -303 241 1 2 8
 ATOM 1179 CD1 LEU 158 -1.212 18.826 46.736 1.000 16.21
 ANISOU 1179 CD1 LEU 158 1224 2249 2685 -111 41 -2 3 9
 ATOM 1180 CD2 LEU 158 -0.086 16.736 47.397 1.000 17.17
 ANISOU 1180 CD2 LEU 158 2656 1542 2325 -254 1273 1 7 4
 ATOM 1181 C LEU 158 1.997 20.626 47.048 1.000 11.22
 ANISOU 1181 C LEU 158 1496 1366 1402 110 -304 5
 ATOM 1182 O LEU 158 3.056 20.201 47.539 1.000 11.28
 ANISOU 1182 O LEU 158 1283 1368 1635 20 -262 7 5
 ATOM 1183 N LEU 159 1.234 21.599 47.548 1.000 10.86
 ANISOU 1183 N LEU 159 1103 1744 1278 68 -180 -7 0
 ATOM 1184 CA LEU 159 1.540 22.278 48.797 1.000 11.62
 ANISOU 1184 CA LEU 159 1247 1761 1407 -59 -68 -1 8 0
 ATOM 1185 CB LEU 159 1.494 23.802 48.640 1.000 12.44
 ANISOU 1185 CB LEU 159 1624 1747 1354 -209 -73 -3 3
 ATOM 1186 CG LEU 159 1.633 24.635 49.934 1.000 12.83
 ANISOU 1186 CG LEU 159 1600 1698 1576 246 -54 -2 1 5
 ATOM 1187 CD1 LEU 159 2.947 24.435 50.651 1.000 14.28
 ANISOU 1187 CD1 LEU 159 2019 2250 1158 177 -292 1 0 4
 ATOM 1188 CD2 LEU 159 1.442 26.134 49.640 1.000 13.33
 ANISOU 1188 CD2 LEU 159 1802 1721 1543 87 -87 -2 0
 ATOM 1189 C LEU 159 0.537 21.846 49.868 1.000 11.24
 ANISOU 1189 C LEU 159 1393 1474 1404 -174 -9 -2 7 1
 ATOM 1190 O LEU 159 -0.665 21.940 49.620 1.000 13.70

- 129 -

ANISOU 1190 O LEU 159 1354 2395 1457 -328 34 -2 6 9
 ATOM 1191 N ARG 160 1.013 21.385 51.010 1.000 14.5 9
 ANISOU 1191 N ARG 160 1737 2569 1239 -390 -128 -2 2 4
 ATOM 1192 CA ARG 160 0.158 21.030 52.153 1.000 13.9 4
 ANISOU 1192 CA ARG 160 1265 2631 1402 157 -137 9 2
 ATOM 1193 CB ARG 160 0.161 19.528 52.343 1.000 18.2 0
 ANISOU 1193 CB ARG 160 1932 2645 2338 -301 32 1 9 3
 ATOM 1194 CG ARG 160 -0.423 18.661 51.252 1.000 25.1 2
 ANISOU 1194 CG ARG 160 3451 2902 3191 -653 -787 2 3
 ATOM 1195 CD ARG 160 -0.765 17.301 51.831 1.000 31.9 8
 ANISOU 1195 CD ARG 160 4825 3598 3729 -1994 -905 3 2 1
 ATOM 1196 NE ARG 160 -1.284 16.322 50.896 1.000 26.1 5
 ANISOU 1196 NE ARG 160 3392 2957 3587 -739 -1056 3 1 0
 ATOM 1197 CZ ARG 160 -0.970 15.044 50.779 1.000 25.3 0
 ANISOU 1197 CZ ARG 160 3195 3390 3028 94 -785 2 9 5
 ATOM 1198 NH1 ARG 160 -0.063 14.433 51.552 1.000 31.2 6
 ANISOU 1198 NH1 ARG 160 3654 4142 4080 -629 -1089 2 0 5 4
 ATOM 1199 NH2 ARG 160 -1.572 14.308 49.850 1.000 28.8 2
 ANISOU 1199 NH2 ARG 160 4020 3122 3807 -13 -966 -9 0
 ATOM 1200 C ARG 160 0.649 21.669 53.447 1.000 15.1 2
 ANISOU 1200 C ARG 160 1649 2863 1232 104 -66 1 2 5
 ATOM 1201 O ARG 160 1.804 21.556 53.863 1.000 17.0 9
 ANISOU 1201 O ARG 160 1291 3411 1791 -400 74 -8 1 2
 ATOM 1202 N PHE 161 -0.258 22.369 54.114 1.000 14.9 5
 ANISOU 1202 N PHE 161 1512 2506 1660 -253 -8 -1 4 6
 ATOM 1203 CA PHE 161 -0.036 22.949 55.427 1.000 13.2 7
 ANISOU 1203 CA PHE 161 1600 1681 1760 -9 -249 -4 1
 ATOM 1204 CB PHE 161 -0.587 24.381 55.472 1.000 16.8 2
 ANISOU 1204 CB PHE 161 1594 1947 2851 384 58 6 4
 ATOM 1205 CG PHE 161 -0.317 25.109 56.771 1.000 22.5 6
 ANISOU 1205 CG PHE 161 2464 2424 3684 -39 790 -1 0 6 7
 ATOM 1206 CD1 PHE 161 -1.175 25.010 57.849 1.000 26.0 3
 ANISOU 1206 CD1 PHE 161 3353 2919 3620 267 1106 -7 0 2
 ATOM 1207 CD2 PHE 161 0.822 25.901 56.885 1.000 25.3 4
 ANISOU 1207 CD2 PHE 161 2353 3265 4011 -179 -161 -7 3 8
 ATOM 1208 CE1 PHE 161 -0.943 25.660 59.051 1.000 30.5 0
 ANISOU 1208 CE1 PHE 161 4784 3324 3481 -972 1456 -6 2 0
 ATOM 1209 CE2 PHE 161 1.061 26.553 58.080 1.000 26.1 0
 ANISOU 1209 CE2 PHE 161 2546 3067 4302 -129 281 -1 1 2 7
 ATOM 1210 CZ PHE 161 0.199 26.438 59.164 1.000 30.0 6
 ANISOU 1210 CZ PHE 161 3839 3197 4386 -152 774 -6 7 7
 ATOM 1211 C PHE 161 -0.737 22.073 56.447 1.000 13.9 3
 ANISOU 1211 C PHE 161 1842 1946 1503 -334 -277 -2 4 0
 ATOM 1212 O PHE 161 -1.916 21.843 56.270 1.000 18.2 6
 ANISOU 1212 O PHE 161 2000 3277 1662 -744 -399 4 7 5
 ATOM 1213 N ARG 162 -0.090 21.631 57.503 1.000 16.2 9
 ANISOU 1213 N ARG 162 2063 2516 1610 -937 -523 7 7
 ATOM 1214 CA ARG 162 -0.635 20.719 58.483 1.000 15.6 2
 ANISOU 1214 CA ARG 162 1772 2512 1650 -519 -266 7 6
 ATOM 1215 C ARG 162 -0.476 21.312 59.890 1.000 17.4 8
 ANISOU 1215 C ARG 162 1855 3131 1656 -603 -186 -7 6
 ATOM 1216 O ARG 162 0.609 21.734 60.251 1.000 17.2 3
 ANISOU 1216 O ARG 162 1928 3063 1557 -771 -42 -1 6 0
 ATOM 1217 CB ARG 162 0.081 19.374 58.458 1.000 21.9 9
 ANISOU 1217 CB ARG 162 3309 2318 2727 -272 -737 -2 2
 ATOM 1218 CG ARG 162 -0.573 18.322 59.348 1.000 26.0 7
 ANISOU 1218 CG ARG 162 3488 2375 4041 489 655 2 8 0
 ATOM 1219 CD ARG 162 -0.231 16.896 58.886 1.000 25.8 5
 ANISOU 1219 CD ARG 162 3106 2221 4495 418 -2 2 3 9
 ATOM 1220 NE ARG 162 -0.943 15.916 59.698 1.000 28.8 3
 ANISOU 1220 NE ARG 162 4379 2437 4139 -181 332 -1 7 7

- 130 -

ATOM	1221	CZ	ARG	162	-0.642	14.638	59.879	1.000	27.99
ANISOU	1221	CZ	ARG	162	4271	2497	3868	-179	962 8 4
ATOM	1222	NH1	ARG	162	0.429	14.119	59.273	1.000	26.61
ANISOU	1222	NH1	ARG	162	3200	3167	3742	-91	-126 -2 6 8
ATOM	1223	NH2	ARG	162	-1.408	13.883	60.658	1.000	34.20
ANISOU	1223	NH2	ARG	162	3807	3522	5663	-986	702 7 8 0
ATOM	1224	N	TYR	163	-1.570	21.296	60.622	1.000	16.77
ANISOU	1224	N	TYR	163	1803	2865	1705	-484	-194 8 4
ATOM	1225	CA	TYR	163	-1.627	21.749	61.997	1.000	16.73
ANISOU	1225	CA	TYR	163	1819	2770	1766	-692	-51 4 0
ATOM	1226	CB	TYR	163	-2.712	22.804	62.116	1.000	18.99
ANISOU	1226	CB	TYR	163	2479	2560	2175	-427	-303 -2 1 4
ATOM	1227	CG	TYR	163	-3.173	23.206	63.488	1.000	23.52
ANISOU	1227	CG	TYR	163	2573	3821	2544	-16	-335 -8 6 8
ATOM	1228	CD1	TYR	163	-2.316	23.848	64.367	1.000	31.80
ANISOU	1228	CD1	TYR	163	3613	5005	3466	-1151	304 -2 3 3 8
ATOM	1229	CE1	TYR	163	-2.731	24.222	65.625	1.000	40.74
ANISOU	1229	CE1	TYR	163	5855	5676	3950	-1906	976 -3 1 1 6
ATOM	1230	CD2	TYR	163	-4.459	22.965	63.931	1.000	32.55
ANISOU	1230	CD2	TYR	163	3307	5654	3408	-1066	639 -2 3 4 0
ATOM	1231	CE2	TYR	163	-4.902	23.332	65.189	1.000	42.99
ANISOU	1231	CE2	TYR	163	5626	6630	4080	-2352	1989 -2 9 4 9
ATOM	1232	CZ	TYR	163	-4.017	23.960	66.025	1.000	42.52
ANISOU	1232	CZ	TYR	163	6281	5799	4075	-1721	1943 -3 7 1 4
ATOM	1233	OH	TYR	163	-4.380	24.351	67.274	1.000	48.87
ANISOU	1233	OH	TYR	163	8167	6831	3569	-269	1801 -3 0 5 2
ATOM	1234	C	TYR	163	-1.935	20.551	62.896	1.000	17.90
ANISOU	1234	C	TYR	163	2872	2353	1575	-894	-465 -1 7 3
ATOM	1235	O	TYR	163	-2.933	19.858	62.653	1.000	18.12
ANISOU	1235	O	TYR	163	2694	2130	2060	-732	-615 6 7
ATOM	1236	N	PHE	164	-1.112	20.326	63.898	1.000	18.32
ANISOU	1236	N	PHE	164	2516	2621	1826	-614	-402 -9 0
ATOM	1237	CA	PHE	164	-1.340	19.381	64.984	1.000	23.44
ANISOU	1237	CA	PHE	164	4176	2692	2038	-727	-669 2 1 9
ATOM	1238	CB	PHE	164	-0.073	18.617	65.327	1.000	26.02
ANISOU	1238	CB	PHE	164	4594	2824	2470	-459	-822 3 7 9
ATOM	1239	CG	PHE	164	0.407	17.669	64.231	1.000	29.00
ANISOU	1239	CG	PHE	164	4118	3639	3263	-518	-427 -2 5 4
ATOM	1240	CD1	PHE	164	1.224	18.118	63.205	1.000	27.11
ANISOU	1240	CD1	PHE	164	3040	4013	3249	-198	-821 4
ATOM	1241	CD2	PHE	164	0.051	16.332	64.240	1.000	28.37
ANISOU	1241	CD2	PHE	164	3935	3139	3704	472	30 -6 4
ATOM	1242	CE1	PHE	164	1.657	17.248	62.223	1.000	28.13
ANISOU	1242	CE1	PHE	164	2730	3926	4034	-43	-229 6
ATOM	1243	CE2	PHE	164	0.459	15.464	63.250	1.000	31.71
ANISOU	1243	CE2	PHE	164	4719	3694	3635	-293	657 -3 8 3
ATOM	1244	CZ	PHE	164	1.276	15.924	62.234	1.000	30.26
ANISOU	1244	CZ	PHE	164	3827	3808	3862	0	300 1 2 6
ATOM	1245	C	PHE	164	-1.775	20.160	66.228	1.000	24.65
ANISOU	1245	C	PHE	164	3541	4049	1777	-1025	-455 3 7
ATOM	1246	O	PHE	164	-0.889	20.713	66.885	1.000	25.54
ANISOU	1246	O	PHE	164	3520	4167	2019	-921	-440 -2 5 7
ATOM	1247	N	PRO	165	-3.058	20.293	66.527	1.000	32.24
ANISOU	1247	N	PRO	165	3641	5095	3513	-1894	266 -6 8 0
ATOM	1248	CA	PRO	165	-3.486	21.012	67.720	1.000	32.98
ANISOU	1248	CA	PRO	165	3570	5737	3225	-1271	397 -3 2 2
ATOM	1249	C	PRO	165	-2.854	20.429	68.986	1.000	38.48
ANISOU	1249	C	PRO	165	4355	6808	3457	-1872	40 3 4 3
ATOM	1250	O	PRO	165	-2.551	19.230	69.034	1.000	53.87
ANISOU	1250	O	PRO	165	9948	7012	3507	-959	692 1 7 5 0
ATOM	1251	CB	PRO	165	-5.001	20.820	67.769	1.000	37.76

- 131 -

ANISOU	1251	CB	PRO	165	3640	6479	4227	-1488	380	-717
ATOM	1252	CG	PRO	165	-5.417	20.048	66.569	1.000	36.16	
ANISOU	1252	CG	PRO	165	3341	6449	3948	-518	-349	-398
ATOM	1253	CD	PRO	165	-4.197	19.816	65.734	1.000	35.70	
ANISOU	1253	CD	PRO	165	3440	6296	3828	-1656	-5	-604
ATOM	1254	N	LEU	178	4.459	8.087	66.987	1.000	36.23	
ANISOU	1254	N	LEU	178	4509	3338	5918	-26	1216	1175
ATOM	1255	CA	LEU	178	4.994	9.117	66.116	1.000	28.63	
ANISOU	1255	CA	LEU	178	3397	3170	4312	377	1344	401
ATOM	1256	CB	LEU	178	5.882	8.534	65.027	1.000	30.08	
ANISOU	1256	CB	LEU	178	3497	3245	4688	760	752	-620
ATOM	1257	CG	LEU	178	7.245	7.948	65.348	1.000	29.43	
ANISOU	1257	CG	LEU	178	3557	2950	4674	667	371	-979
ATOM	1258	CD1	LEU	178	7.859	7.367	64.073	1.000	32.13	
ANISOU	1258	CD1	LEU	178	2972	4524	4713	586	810	-790
ATOM	1259	CD2	LEU	178	8.208	8.964	65.937	1.000	41.71	
ANISOU	1259	CD2	LEU	178	5303	3695	6850	356	-1656	-1154
ATOM	1260	C	LEU	178	3.885	9.909	65.420	1.000	27.18	
ANISOU	1260	C	LEU	178	2107	3534	4686	-175	1776	833
ATOM	1261	O	LEU	178	2.845	9.351	65.086	1.000	39.60	
ANISOU	1261	O	LEU	178	2407	4624	8016	-1253	1290	2183
ATOM	1262	N	ARG	179	4.128	11.200	65.160	1.000	25.65	
ANISOU	1262	N	ARG	179	2220	3437	4089	-216	878	741
ATOM	1263	CA	ARG	179	3.231	11.973	64.321	1.000	25.04	
ANISOU	1263	CA	ARG	179	1860	3289	4365	69	641	15
ATOM	1264	C	ARG	179	3.297	11.572	62.852	1.000	24.51	
ANISOU	1264	C	ARG	179	2158	2721	4434	39	99	-89
ATOM	1265	O	ARG	179	2.295	11.687	62.139	1.000	28.60	
ANISOU	1265	O	ARG	179	2545	3242	5079	441	-332	-256
ATOM	1266	CB	ARG	179	3.517	13.480	64.451	1.000	28.58	
ANISOU	1266	CB	ARG	179	3980	3317	3561	-110	-843	57
ATOM	1267	CG	ARG	179	2.936	14.092	65.724	1.000	30.01	
ANISOU	1267	CG	ARG	179	3817	3725	3862	57	-957	-372
ATOM	1268	CD	ARG	179	3.307	15.570	65.757	1.000	31.51	
ANISOU	1268	CD	ARG	179	4457	3675	3840	90	-1514	-338
ATOM	1269	NE	ARG	179	2.925	16.126	67.058	1.000	37.82	
ANISOU	1269	NE	ARG	179	7035	3190	4144	153	-310	-15
ATOM	1270	CZ	ARG	179	2.897	17.425	67.292	1.000	39.43	
ANISOU	1270	CZ	ARG	179	8420	3029	3532	-479	580	400
ATOM	1271	NH1	ARG	179	3.213	18.286	66.331	1.000	59.73	
ANISOU	1271	NH1	ARG	179	11745	4676	6273	-1045	3177	1722
ATOM	1272	NH2	ARG	179	2.548	17.896	68.457	1.000	33.13	
ANISOU	1272	NH2	ARG	179	5661	3832	3094	275	-1463	-173
ATOM	1273	N	MET	180	4.455	11.099	62.424	1.000	21.43	
ANISOU	1273	N	MET	180	2013	2457	3674	-395	108	-222
ATOM	1274	CA	MET	180	4.695	10.539	61.108	1.000	20.07	
ANISOU	1274	CA	MET	180	2346	1965	3315	-349	-300	151
ATOM	1275	C	MET	180	5.802	9.482	61.182	1.000	17.33	
ANISOU	1275	C	MET	180	2251	2080	2254	-332	-86	337
ATOM	1276	O	MET	180	6.894	9.757	61.677	1.000	18.52	
ANISOU	1276	O	MET	180	2237	2019	2781	-398	-79	52
ATOM	1277	CB	MET	180	5.041	11.646	60.136	1.000	22.64	
ANISOU	1277	CB	MET	180	2571	2321	3709	-197	-549	683
ATOM	1278	CG	MET	180	5.065	11.367	58.678	1.000	27.90	
ANISOU	1278	CG	MET	180	3918	3095	3588	-453	-654	913
ATOM	1279	SD	MET	180	4.945	12.838	57.629	1.000	25.01	
ANISOU	1279	SD	MET	180	2936	2942	3626	-399	124	851
ATOM	1280	CE	MET	180	4.385	12.010	56.147	1.000	37.00	
ANISOU	1280	CE	MET	180	5917	3450	4690	-258	-2680	1204
ATOM	1281	N	ALA	181	5.467	8.295	60.680	1.000	16.99	
ANISOU	1281	N	ALA	181	2144	2139	2174	-90	-558	299

- 132 -

ATOM 1282 CA ALA 181 6.396 7.168 60.676 1.000 16.12
 ANISOU 1282 CA ALA 181 2275 1958 1890 -171 -343 6 0 2
 ATOM 1283 CB ALA 181 5.668 5.891 60.279 1.000 20.24
 ANISOU 1283 CB ALA 181 2857 2158 2673 -648 694 1 0 6
 ATOM 1284 C ALA 181 7.576 7.409 59.738 1.000 15.43
 ANISOU 1284 C ALA 181 2223 1717 1925 -315 -369 4 3 2
 ATOM 1285 O ALA 181 7.458 8.198 58.783 1.000 15.49
 ANISOU 1285 O ALA 181 2268 1761 1858 -173 -296 4 3 4
 ATOM 1286 N PRO 182 8.698 6.733 59.986 1.000 16.03
 ANISOU 1286 N PRO 182 2517 1745 1829 32 -78 5 3 1
 ATOM 1287 CD PRO 182 8.983 5.802 61.101 1.000 19.61
 ANISOU 1287 CD PRO 182 2321 2908 2221 -210 -306 1 2 4 0
 ATOM 1288 CA PRO 182 9.865 6.907 59.076 1.000 14.78
 ANISOU 1288 CA PRO 182 2573 1336 1706 -101 -86 2 9 9
 ATOM 1289 CB PRO 182 10.914 5.948 59.649 1.000 16.20
 ANISOU 1289 CB PRO 182 2570 1978 1607 170 -251 7 7
 ATOM 1290 CG PRO 182 10.479 5.713 61.066 1.000 19.28
 ANISOU 1290 CG PRO 182 2301 3071 1952 -199 -245 1 0 0 1
 ATOM 1291 C PRO 182 9.541 6.571 57.627 1.000 14.90
 ANISOU 1291 C PRO 182 2230 1658 1772 -421 -262 3 4 0
 ATOM 1292 O PRO 182 8.920 5.573 57.249 1.000 15.38
 ANISOU 1292 O PRO 182 2301 1587 1957 -467 -482 5 3 9
 ATOM 1293 N HIS 183 9.969 7.460 56.730 1.000 12.28
 ANISOU 1293 N HIS 183 1737 1312 1617 -154 -284 1 5 6
 ATOM 1294 CA HIS 183 9.733 7.354 55.300 1.000 11.90
 ANISOU 1294 CA HIS 183 1413 1495 1614 -254 -351 3 5
 ATOM 1295 CB HIS 183 8.300 7.824 54.922 1.000 12.43
 ANISOU 1295 CB HIS 183 1399 1368 1957 -128 -241 1 1 2
 ATOM 1296 CG HIS 183 8.168 9.314 55.089 1.000 11.36
 ANISOU 1296 CG HIS 183 1349 1369 1600 -367 -296 5 6
 ATOM 1297 CD2 HIS 183 8.259 10.374 54.249 1.000 12.03
 ANISOU 1297 CD2 HIS 183 1684 1296 1589 -43 157 -1 0
 ATOM 1298 ND1 HIS 183 7.989 9.858 56.339 1.000 13.27
 ANISOU 1298 ND1 HIS 183 1901 1439 1700 -65 267 1 9 3
 ATOM 1299 CE1 HIS 183 7.943 11.187 56.244 1.000 12.43
 ANISOU 1299 CE1 HIS 183 1939 1490 1296 77 -244 1 5 0
 ATOM 1300 NE2 HIS 183 8.101 11.515 54.992 1.000 11.04
 ANISOU 1300 NE2 HIS 183 1560 1437 1199 215 -232 4 8
 ATOM 1301 C HIS 183 10.749 8.176 54.515 1.000 12.27
 ANISOU 1301 C HIS 183 1446 1639 1577 -303 -282 -6 7
 ATOM 1302 O HIS 183 11.433 9.032 55.064 1.000 12.94
 ANISOU 1302 O HIS 183 1496 1915 1505 -558 -292 1 5
 ATOM 1303 N TYR 184 10.849 7.907 53.215 1.000 10.61
 ANISOU 1303 N TYR 184 1453 1027 1552 -41 -380 1 1 0
 ATOM 1304 CA TYR 184 11.483 8.800 52.256 1.000 11.36
 ANISOU 1304 CA TYR 184 1475 1104 1738 -71 -264 1 7 8
 ATOM 1305 CB TYR 184 12.628 8.151 51.481 1.000 11.79
 ANISOU 1305 CB TYR 184 1631 1114 1734 -62 -197 3 4
 ATOM 1306 CG TYR 184 12.368 6.907 50.677 1.000 11.29
 ANISOU 1306 CG TYR 184 1680 921 1688 225 -893 1 7 4
 ATOM 1307 CD1 TYR 184 12.156 5.659 51.268 1.000 11.76
 ANISOU 1307 CD1 TYR 184 1663 927 1879 388 -487 1 9 0
 ATOM 1308 CE1 TYR 184 11.911 4.526 50.492 1.000 12.64
 ANISOU 1308 CE1 TYR 184 1960 878 1964 173 -40 1 8 2
 ATOM 1309 CD2 TYR 184 12.333 6.949 49.279 1.000 11.13
 ANISOU 1309 CD2 TYR 184 1252 1302 1674 109 -283 9 3
 ATOM 1310 CE2 TYR 184 12.102 5.834 48.502 1.000 12.93
 ANISOU 1310 CE2 TYR 184 1944 1422 1546 49 -384 7 3
 ATOM 1311 CZ TYR 184 11.898 4.611 49.121 1.000 13.14
 ANISOU 1311 CZ TYR 184 1717 1304 1972 30 -611 6 7
 ATOM 1312 OH TYR 184 11.663 3.490 48.343 1.000 15.45

- 133 -

ANISOU	1312	OH	TYR	184	2028	1471	2373	42	-476	-2	4	7
ATOM	1313	C	TYR	184	10.447	9.390	51.314	1.000	11.50			
ANISOU	1313	C	TYR	184	1445	1215	1709	-187	-201	3	4	8
ATOM	1314	O	TYR	184	9.362	8.797	51.089	1.000	11.75			
ANISOU	1314	O	TYR	184	1305	1308	1853	-106	-171	4	2	7
ATOM	1315	N	ASP	185	10.784	10.557	50.743	1.000	10.79			
ANISOU	1315	N	ASP	185	1581	1069	1449	-141	-132	1	1	8
ATOM	1316	CA	ASP	185	9.861	11.218	49.815	1.000	9.10			
ANISOU	1316	CA	ASP	185	1089	1093	1277	-326	23	2	0	6
ATOM	1317	CB	ASP	185	9.934	12.743	49.886	1.000	10.13			
ANISOU	1317	CB	ASP	185	1427	1095	1327	-298	-178	1	7	7
ATOM	1318	CG	ASP	185	9.540	13.388	51.185	1.000	11.79			
ANISOU	1318	CG	ASP	185	1797	1350	1333	-250	-149	1	1	
ATOM	1319	OD1	ASP	185	9.681	14.638	51.278	1.000	13.79			
ANISOU	1319	OD1	ASP	185	2050	1316	1875	135	-52	-2	6	
ATOM	1320	OD2	ASP	185	9.114	12.755	52.189	1.000	13.31			
ANISOU	1320	OD2	ASP	185	1805	1848	1405	-411	-63	1	0	5
ATOM	1321	C	ASP	185	10.098	10.759	48.371	1.000	9.44			
ANISOU	1321	C	ASP	185	1036	1150	1401	-309	-26	1	0	0
ATOM	1322	O	ASP	185	11.234	10.469	48.005	1.000	10.64			
ANISOU	1322	O	ASP	185	1167	1376	1500	-127	-35	-2	0	6
ATOM	1323	N	LEU	186	9.038	10.684	47.568	1.000	10.09			
ANISOU	1323	N	LEU	186	1211	1186	1437	-272	-177	-5	8	
ATOM	1324	CA	LEU	186	9.124	10.312	46.161	1.000	10.60			
ANISOU	1324	CA	LEU	186	1641	986	1401	-239	-52	-4	4	
ATOM	1325	CB	LEU	186	8.030	9.295	45.798	1.000	11.32			
ANISOU	1325	CB	LEU	186	1652	929	1721	-111	17	-4	7	9
ATOM	1326	CG	LEU	186	7.989	7.977	46.602	1.000	12.60			
ANISOU	1326	CG	LEU	186	1408	1039	2340	-263	-200	-1	6	6
ATOM	1327	CD1	LEU	186	6.896	7.064	46.028	1.000	16.64			
ANISOU	1327	CD1	LEU	186	1900	1373	3049	-634	-398	-1	3	5
ATOM	1328	CD2	LEU	186	9.356	7.332	46.629	1.000	13.84			
ANISOU	1328	CD2	LEU	186	1438	1245	2575	-155	443	2	8	3
ATOM	1329	C	LEU	186	9.024	11.521	45.223	1.000	10.90			
ANISOU	1329	C	LEU	186	1327	1211	1603	-3	-451	1	6	4
ATOM	1330	O	LEU	186	8.768	11.406	44.031	1.000	13.60			
ANISOU	1330	O	LEU	186	2067	1608	1494	-211	-321	1	0	3
ATOM	1331	N	SER	187	9.264	12.705	45.734	1.000	10.71			
ANISOU	1331	N	SER	187	1546	1129	1393	-76	-282	3	1	8
ATOM	1332	CA	SER	187	9.401	13.943	44.998	1.000	10.49			
ANISOU	1332	CA	SER	187	1427	1191	1370	195	-107	4	8	8
ATOM	1333	CB	SER	187	9.221	15.103	46.002	1.000	10.56			
ANISOU	1333	CB	SER	187	1105	1048	1857	298	161	5	3	2
ATOM	1334	OG	SER	187	10.430	14.918	46.726	1.000	13.01			
ANISOU	1334	OG	SER	187	1343	1432	2169	-132	-295	2	0	1
ATOM	1335	C	SER	187	10.774	14.062	44.336	1.000	10.47			
ANISOU	1335	C	SER	187	1447	862	1669	135	-3	1	4	5
ATOM	1336	O	SER	187	11.684	13.246	44.513	1.000	10.54			
ANISOU	1336	O	SER	187	1577	799	1629	183	-91	-7	7	
ATOM	1337	N	MET	188	10.962	15.095	43.502	1.000	9.78			
ANISOU	1337	N	MET	188	1419	978	1318	147	44	7	4	
ATOM	1338	CA	MET	188	12.267	15.584	43.065	1.000	9.94			
ANISOU	1338	CA	MET	188	1394	942	1441	182	58	3	7	
ATOM	1339	CB	MET	188	12.128	16.543	41.891	1.000	10.89			
ANISOU	1339	CB	MET	188	1523	840	1774	98	48	2	2	7
ATOM	1340	CG	MET	188	13.385	17.258	41.470	1.000	11.40			
ANISOU	1340	CG	MET	188	1403	1172	1756	46	-51	2	1	4
ATOM	1341	SD	MET	188	14.687	16.134	40.891	1.000	12.71			
ANISOU	1341	SD	MET	188	1619	1272	1940	139	137	1	9	8
ATOM	1342	CE	MET	188	16.061	17.267	40.790	1.000	13.86			
ANISOU	1342	CE	MET	188	1862	1399	2003	-2	911	-9	0	

- 134 -

ATOM	1343	C	MET	188	12.946	16.217	44.291	1.000	12.13
ANISOU	1343	C	MET	188	1325	1586	1698	169	-18 -285
ATOM	1344	O	MET	188	13.971	15.727	44.804	1.000	11.52
ANISOU	1344	O	MET	188	1288	1553	1535	144	132 8 7
ATOM	1345	N	VAL	189	12.362	17.290	44.838	1.000	10.00
ANISOU	1345	N	VAL	189	1290	1217	1292	53	-175 6
ATOM	1346	CA	VAL	189	12.745	17.894	46.099	1.000	9.70
ANISOU	1346	CA	VAL	189	1209	1057	1420	-212	-45 -19
ATOM	1347	CB	VAL	189	13.618	19.154	45.979	1.000	9.97
ANISOU	1347	CB	VAL	189	1288	1103	1398	-238	129 189
ATOM	1348	CG1	VAL	189	14.953	18.837	45.266	1.000	13.45
ANISOU	1348	CG1	VAL	189	1334	1410	2368	-236	390 143
ATOM	1349	CG2	VAL	189	12.899	20.289	45.264	1.000	12.24
ANISOU	1349	CG2	VAL	189	1715	1242	1693	-25	150 295
ATOM	1350	C	VAL	189	11.469	18.245	46.871	1.000	10.10
ANISOU	1350	C	VAL	189	1089	1600	1149	-456	-156 -73
ATOM	1351	O	VAL	189	10.405	18.399	46.250	1.000	9.53
ANISOU	1351	O	VAL	189	1153	1249	1217	-222	-190 8
ATOM	1352	N	THR	190	11.609	18.327	48.187	1.000	8.66
ANISOU	1352	N	THR	190	1273	894 1123	15	-202	127
ATOM	1353	CA	THR	190	10.565	18.771	49.091	1.000	9.64
ANISOU	1353	CA	THR	190	1350	1167	1147	-11	-228 -99
ATOM	1354	CB	THR	190	10.194	17.699	50.132	1.000	10.69
ANISOU	1354	CB	THR	190	1231	1196	1635	-300	121 -54
ATOM	1355	OG1	THR	190	9.662	16.586	49.501	1.000	12.45
ANISOU	1355	OG1	THR	190	1333	1341	2055	-140	-258 -48
ATOM	1356	CG2	THR	190	9.038	18.131	51.019	1.000	13.59
ANISOU	1356	CG2	THR	190	1121	2222	1821	-272	151 -195
ATOM	1357	C	THR	190	11.058	19.976	49.891	1.000	9.23
ANISOU	1357	C	THR	190	1257	1096	1152	-102	-336 -49
ATOM	1358	O	THR	190	12.149	19.867	50.447	1.000	10.54
ANISOU	1358	O	THR	190	1322	1292	1390	-5	-359 -122
ATOM	1359	N	LEU	191	10.313	21.064	49.978	1.000	10.23
ANISOU	1359	N	LEU	191	1319	1167	1401	-71	-177 -133
ATOM	1360	CA	LEU	191	10.691	22.241	50.770	1.000	10.19
ANISOU	1360	CA	LEU	191	1259	1176	1438	0	-294 -142
ATOM	1361	CB	LEU	191	10.604	23.511	49.910	1.000	11.52
ANISOU	1361	CB	LEU	191	1203	1185	1990	-118	-601 32
ATOM	1362	CG	LEU	191	11.897	23.898	49.167	1.000	13.23
ANISOU	1362	CG	LEU	191	1898	1710	1419	-391	-358 97
ATOM	1363	CD1	LEU	191	12.333	22.794	48.218	1.000	15.25
ANISOU	1363	CD1	LEU	191	1685	2018	2091	-476	-214 -305
ATOM	1364	CD2	LEU	191	11.717	25.231	48.448	1.000	17.46
ANISOU	1364	CD2	LEU	191	2310	2044	2281	-14	17604
ATOM	1365	C	LEU	191	9.798	22.328	52.006	1.000	11.93
ANISOU	1365	C	LEU	191	1275	1677	1579	56	-190 -372
ATOM	1366	O	LEU	191	8.560	22.262	51.868	1.000	13.49
ANISOU	1366	O	LEU	191	1276	2173	1676	1	-192 -601
ATOM	1367	N	ILE	192	10.394	22.483	53.190	1.000	11.06
ANISOU	1367	N	ILE	192	1115	1603	1487	-111	-92 -108
ATOM	1368	CA	ILE	192	9.671	22.539	54.443	1.000	11.13
ANISOU	1368	CA	ILE	192	1071	1638	1521	11	-173 -149
ATOM	1369	CB	ILE	192	9.927	21.304	55.330	1.000	12.94
ANISOU	1369	CB	ILE	192	2099	1586	1232	-65	-9 -233
ATOM	1370	CG2	ILE	192	9.221	21.428	56.673	1.000	16.06
ANISOU	1370	CG2	ILE	192	2479	1983	1641	-206	426 -215
ATOM	1371	CG1	ILE	192	9.512	20.028	54.590	1.000	15.51
ANISOU	1371	CG1	ILE	192	2633	1658	1601	-400	-48 -175
ATOM	1372	CD1	ILE	192	9.845	18.765	55.339	1.000	25.71
ANISOU	1372	CD1	ILE	192	5869	1608	2290	-175	-1566 -301
ATOM	1373	C	ILE	192	9.966	23.809	55.253	1.000	11.47

- 135 -

ANISOU 1373 C ILE 192 1330 1603 1427 -4 -222 -1 2 2
 ATOM 1374 O ILE 192 11.123 24.106 55.567 1.000 13.33
 ANISOU 1374 O ILE 192 1344 1738 1981 -96 -289 -2 1 9
 ATOM 1375 N GLN 193 8.904 24.525 55.602 1.000 15.78
 ANISOU 1375 N GLN 193 1316 2462 2219 -64 -5 -9 7 5
 ATOM 1376 CA GLN 193 8.987 25.653 56.533 1.000 14.56
 ANISOU 1376 CA GLN 193 1582 1858 2091 212 -304 -5 2 9
 ATOM 1377 CB GLN 193 8.449 26.975 56.020 1.000 20.03
 ANISOU 1377 CB GLN 193 2226 2203 3180 318 -329 1 4 2
 ATOM 1378 CG GLN 193 9.203 27.684 54.914 1.000 23.86
 ANISOU 1378 CG GLN 193 3399 2492 3174 313 45 2 8 0
 ATOM 1379 CD GLN 193 8.665 29.079 54.675 1.000 22.92
 ANISOU 1379 CD GLN 193 3250 2363 3097 78 -477 2 0 5
 ATOM 1380 OE1 GLN 193 7.603 29.292 54.099 1.000 27.68
 ANISOU 1380 OE1 GLN 193 4175 3310 3031 552 -1214 2 9
 ATOM 1381 NE2 GLN 193 9.411 30.075 55.134 1.000 27.01
 ANISOU 1381 NE2 GLN 193 3187 2667 4408 -440 124 1 7
 ATOM 1382 C GLN 193 8.216 25.265 57.804 1.000 15.14
 ANISOU 1382 C GLN 193 1945 1827 1982 136 -174 -7 2 2
 ATOM 1383 O GLN 193 7.147 24.662 57.714 1.000 27.80
 ANISOU 1383 O GLN 193 2523 6225 1817 -1586 -592 2 3 5
 ATOM 1384 N GLN 194 8.714 25.552 58.978 1.000 19.80
 ANISOU 1384 N GLN 194 2994 2502 2025 -632 -752 3 3
 ATOM 1385 CA GLN 194 8.100 25.080 60.213 1.000 22.89
 ANISOU 1385 CA GLN 194 3961 2626 2110 493 -20 5 2
 ATOM 1386 C GLN 194 7.763 26.236 61.141 1.000 27.79
 ANISOU 1386 C GLN 194 4886 2757 2916 823 25 -2 6 2
 ATOM 1387 O GLN 194 8.424 27.258 60.983 1.000 30.03
 ANISOU 1387 O GLN 194 4727 3168 3516 368 -259 -9 1 0
 ATOM 1388 CB GLN 194 9.086 24.170 60.950 1.000 23.97
 ANISOU 1388 CB GLN 194 3952 3133 2021 846 483 3 5 2
 ATOM 1389 CG GLN 194 9.398 22.835 60.314 1.000 21.94
 ANISOU 1389 CG GLN 194 2740 3238 2358 683 -182 -1 0
 ATOM 1390 CD GLN 194 10.546 22.148 61.052 1.000 20.51
 ANISOU 1390 CD GLN 194 2450 3433 1911 509 -321 -4 2 9
 ATOM 1391 OE1 GLN 194 11.707 22.142 60.627 1.000 20.80
 ANISOU 1391 OE1 GLN 194 2245 2996 2662 -171 -382 -6 8 1
 ATOM 1392 NE2 GLN 194 10.223 21.585 62.197 1.000 24.91
 ANISOU 1392 NE2 GLN 194 2539 3902 3023 210 -365 7 6 0
 ATOM 1393 N THR 195 6.817 26.035 62.030 1.000 32.47
 ANISOU 1393 N THR 195 5716 2729 3891 1095 1056 -6 1 6
 ATOM 1394 CA THR 195 6.588 26.708 63.282 1.000 35.83
 ANISOU 1394 CA THR 195 6329 3539 3748 1011 999 -7 2 2
 ATOM 1395 CB THR 195 5.263 27.492 63.357 1.000 37.96
 ANISOU 1395 CB THR 195 5756 4304 4365 647 2095 -1 1 5 1
 ATOM 1396 OG1 THR 195 4.191 26.576 63.604 1.000 48.36
 ANISOU 1396 OG1 THR 195 6874 6076 5423 -806 2581 -1 8 4 2
 ATOM 1397 CG2 THR 195 4.958 28.175 62.033 1.000 44.54
 ANISOU 1397 CG2 THR 195 2944 7471 6510 -872 -963 6 2 1
 ATOM 1398 C THR 195 6.590 25.684 64.429 1.000 48.86
 ANISOU 1398 C THR 195 10133 4924 3508 -321 -1356 -2 2 1
 ATOM 1399 O THR 195 6.122 24.544 64.293 1.000 64.12
 ANISOU 1399 O THR 195 13267 4150 6945 -264 -4541 1 6 8 2
 ATOM 1400 N PHE 201 12.035 21.374 72.205 1.000 71.12
 ANISOU 1400 N PHE 201 13961 9034 4028 -5932 -1658 -1 7 4 1
 ATOM 1401 CA PHE 201 11.775 20.053 71.629 1.000 49.44
 ANISOU 1401 CA PHE 201 7918 7543 3326 -3128 1317 -1 4 8 8
 ATOM 1402 CB PHE 201 10.469 19.464 72.181 1.000 47.85
 ANISOU 1402 CB PHE 201 7119 6892 4168 -1869 1937 -1 8 9 9
 ATOM 1403 CG PHE 201 10.130 18.113 71.545 1.000 46.41
 ANISOU 1403 CG PHE 201 6643 6596 4396 -2038 1879 -1 4 9 7

- 136 -

ATOM 1404 CD1 PHE 201 10.738 16.954 71.991 1.000 50.03
 ANISOU 1404 CD1 PHE 201 7982 6634 4393 -2326 1092 -991
 ATOM 1405 CD2 PHE 201 9.220 18.001 70.513 1.000 42.63
 ANISOU 1405 CD2 PHE 201 5458 6427 4313 -1097 2449 -2268
 ATOM 1406 CE1 PHE 201 10.434 15.739 71.417 1.000 49.95
 ANISOU 1406 CE1 PHE 201 8275 6464 4240 -2047 227 -716
 ATOM 1407 CE2 PHE 201 8.901 16.783 69.934 1.000 41.38
 ANISOU 1407 CE2 PHE 201 6016 5946 3762 -578 2006 -1844
 ATOM 1408 CZ PHE 201 9.515 15.636 70.392 1.000 44.74
 ANISOU 1408 CZ PHE 201 7075 6261 3663 -1063 1020 -975
 ATOM 1409 C PHE 201 11.722 20.110 70.107 1.000 42.42
 ANISOU 1409 C PHE 201 6324 6442 3351 -1964 717 -1441
 ATOM 1410 O PHE 201 11.007 20.941 69.536 1.000 47.79
 ANISOU 1410 O PHE 201 9668 4400 4090 -762 691 -2416
 ATOM 1411 N VAL 202 12.477 19.232 69.449 1.000 34.04
 ANISOU 1411 N VAL 202 4525 5852 2558 -1948 7 -425
 ATOM 1412 CA VAL 202 12.535 19.245 67.993 1.000 25.09
 ANISOU 1412 CA VAL 202 3221 3752 2558 -1041 -182 9 9
 ATOM 1413 CB VAL 202 13.988 19.286 67.489 1.000 22.88
 ANISOU 1413 CB VAL 202 2832 3430 2432 -577 -691 -198
 ATOM 1414 CG1 VAL 202 14.053 19.387 65.965 1.000 26.02
 ANISOU 1414 CG1 VAL 202 3821 3594 2470 -958 35 -277
 ATOM 1415 CG2 VAL 202 14.771 20.443 68.078 1.000 24.69
 ANISOU 1415 CG2 VAL 202 3043 3473 2867 -786 -410 -320
 ATOM 1416 C VAL 202 11.798 18.035 67.421 1.000 20.69
 ANISOU 1416 C VAL 202 3027 2810 2023 -648 58 6 15
 ATOM 1417 O VAL 202 12.288 16.914 67.581 1.000 26.08
 ANISOU 1417 O VAL 202 3294 3219 3396 -136 452 8 8 4
 ATOM 1418 N SER 203 10.662 18.234 66.766 1.000 20.21
 ANISOU 1418 N SER 203 3100 2794 1787 -414 25 -152
 ATOM 1419 CA SER 203 9.820 17.192 66.218 1.000 20.37
 ANISOU 1419 CA SER 203 3149 2709 1884 -355 129 -256
 ATOM 1420 CB SER 203 8.437 17.779 65.896 1.000 24.72
 ANISOU 1420 CB SER 203 2726 4106 2558 -178 369 -1015
 ATOM 1421 OG SER 203 7.841 18.239 67.097 1.000 31.80
 ANISOU 1421 OG SER 203 3328 5782 2974 -457 1175 -1104
 ATOM 1422 C SER 203 10.367 16.524 64.958 1.000 19.13
 ANISOU 1422 C SER 203 2580 2647 2040 -339 170 -244
 ATOM 1423 O SER 203 10.279 15.302 64.832 1.000 17.01
 ANISOU 1423 O SER 203 2311 2625 1527 -414 206 -18
 ATOM 1424 N LEU 204 10.902 17.259 63.998 1.000 16.16
 ANISOU 1424 N LEU 204 2142 1976 2024 71 77 -292
 ATOM 1425 CA LEU 204 11.403 16.679 62.740 1.000 14.07
 ANISOU 1425 CA LEU 204 1670 1626 2049 -22 -24 -283
 ATOM 1426 CB LEU 204 11.269 17.704 61.618 1.000 13.80
 ANISOU 1426 CB LEU 204 1549 1763 1931 -249 -340 -277
 ATOM 1427 CG LEU 204 11.647 17.272 60.212 1.000 14.13
 ANISOU 1427 CG LEU 204 1726 1722 1919 -253 -482 -412
 ATOM 1428 CD1 LEU 204 10.770 16.134 59.680 1.000 18.76
 ANISOU 1428 CD1 LEU 204 2579 2895 1654 -1297 -927 -106
 ATOM 1429 CD2 LEU 204 11.609 18.478 59.255 1.000 16.20
 ANISOU 1429 CD2 LEU 204 1987 2095 2074 65 75 -123
 ATOM 1430 C LEU 204 12.832 16.140 62.885 1.000 14.81
 ANISOU 1430 C LEU 204 1734 1748 2144 9 -199 -250
 ATOM 1431 O LEU 204 13.699 16.853 63.397 1.000 15.52
 ANISOU 1431 O LEU 204 1833 1789 2274 -59 -435 -42
 ATOM 1432 N GLN 205 13.065 14.900 62.469 1.000 14.42
 ANISOU 1432 N GLN 205 1847 1804 1827 189 -120 -153
 ATOM 1433 CA GLN 205 14.288 14.143 62.574 1.000 12.76
 ANISOU 1433 CA GLN 205 1777 1655 1419 43 -347 -113
 ATOM 1434 C GLN 205 14.622 13.434 61.260 1.000 11.12

- 137 -

ANISOU 1434 C GLN 205 1412 1474 1338 49 -468 - 2 1
 ATOM 1435 O GLN 205 13.707 12.927 60.606 1.000 13.97
 ANISOU 1435 O GLN 205 1622 2235 1449 -293 -449 -1 4 7
 ATOM 1436 CB GLN 205 14.164 13.062 63.662 1.000 15.57
 ANISOU 1436 CB GLN 205 2421 1925 1568 341 151 8 3
 ATOM 1437 CG GLN 205 13.863 13.635 65.032 1.000 18.58
 ANISOU 1437 CG GLN 205 3321 2286 1451 689 -129 8 2
 ATOM 1438 CD GLN 205 15.086 14.243 65.680 1.000 24.33
 ANISOU 1438 CD GLN 205 3687 3465 2091 520 -499 -5 7 0
 ATOM 1439 OE1 GLN 205 16.206 13.717 65.549 1.000 29.12
 ANISOU 1439 OE1 GLN 205 3350 3464 4251 14 -270 -1800
 ATOM 1440 NE2 GLN 205 14.840 15.356 66.378 1.000 23.01
 ANISOU 1440 NE2 GLN 205 3055 2465 3225 335 -592 -1 4 0
 ATOM 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63
 ANISOU 1441 N ALA 206 1523 1770 1506 -251 -234 - 6
 ATOM 1442 CA ALA 206 16.335 12.649 59.731 1.000 13.77
 ANISOU 1442 CA ALA 206 1392 2099 1742 -522 -72 -2 9 5
 ATOM 1443 CB ALA 206 16.693 13.519 58.528 1.000 16.34
 ANISOU 1443 CB ALA 206 2034 2494 1682 -603 123 -2 7 7
 ATOM 1444 C ALA 206 17.567 11.813 60.046 1.000 15.92
 ANISOU 1444 C ALA 206 1489 2331 2230 -290 179 -3 4 1
 ATOM 1445 O ALA 206 18.368 12.182 60.908 1.000 15.86
 ANISOU 1445 O ALA 206 1877 1772 2377 150 -356 3 0
 ATOM 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98
 ANISOU 1446 N GLU 207 1981 2086 2383 -335 348 -1 8 6
 ATOM 1447 CA GLU 207 18.938 9.942 59.364 1.000 20.58
 ANISOU 1447 CA GLU 207 2198 1938 3684 -164 490 -1 0
 ATOM 1448 C GLU 207 20.082 10.688 58.681 1.000 18.75
 ANISOU 1448 C GLU 207 1828 2037 3260 272 185 5 5 8
 ATOM 1449 O GLU 207 19.948 10.953 57.503 1.000 18.23
 ANISOU 1449 O GLU 207 1746 2145 3034 52 8 -4 5
 ATOM 1450 CB GLU 207 18.665 8.612 58.676 1.000 25.81
 ANISOU 1450 CB GLU 207 3289 1794 4724 -19 83 -1 3 5
 ATOM 1451 CG GLU 207 19.879 7.737 58.429 1.000 30.08
 ANISOU 1451 CG GLU 207 4102 2221 5105 907 -948 -5 4 6
 ATOM 1452 CD GLU 207 19.429 6.356 57.959 1.000 29.93
 ANISOU 1452 CD GLU 207 5549 2024 3798 1179 -2099 -1 2 3
 ATOM 1453 OE1 GLU 207 19.491 5.471 58.839 1.000 35.14
 ANISOU 1453 OE1 GLU 207 5782 2692 4879 938 -931 8 8 5
 ATOM 1454 OE2 GLU 207 19.037 6.251 56.762 1.000 38.62
 ANISOU 1454 OE2 GLU 207 4955 5608 4109 135 -2494 -3 6 6
 ATOM 1455 N VAL 208 21.146 10.997 59.414 1.000 16.97
 ANISOU 1455 N VAL 208 1926 1974 2549 120 337 8 0 7
 ATOM 1456 CA VAL 208 22.376 11.593 58.902 1.000 17.77
 ANISOU 1456 CA VAL 208 1894 2109 2748 93 500 4 1 1
 ATOM 1457 CB VAL 208 22.455 13.111 59.155 1.000 16.89
 ANISOU 1457 CB VAL 208 2774 2148 1494 -372 -149 5 6 9
 ATOM 1458 CG1 VAL 208 23.652 13.688 58.409 1.000 20.76
 ANISOU 1458 CG1 VAL 208 3214 2150 2526 -423 647 1 4 8
 ATOM 1459 CG2 VAL 208 21.172 13.815 58.720 1.000 16.36
 ANISOU 1459 CG2 VAL 208 3146 1640 1431 25 98 3 5 3
 ATOM 1460 C VAL 208 23.585 10.877 59.507 1.000 20.29
 ANISOU 1460 C VAL 208 1936 2555 3217 11 -58 1 3 2
 ATOM 1461 O VAL 208 23.726 10.829 60.741 1.000 20.74
 ANISOU 1461 O VAL 208 2436 2256 3187 460 206 5 4 4
 ATOM 1462 N GLY 209 24.457 10.295 58.672 1.000 18.94
 ANISOU 1462 N GLY 209 1764 2445 2989 211 -494 1 5
 ATOM 1463 CA GLY 209 25.558 9.508 59.194 1.000 24.01
 ANISOU 1463 CA GLY 209 2171 3040 3910 549 -396 7 0 9
 ATOM 1464 C GLY 209 25.123 8.364 60.082 1.000 25.00
 ANISOU 1464 C GLY 209 2874 3156 3470 1406 772 6 4 9

- 138 -

ATOM 1465 O GLY 209 25.850 7.934 60.991 1.000 35.98
 ANISOU 1465 O GLY 209 4448 3946 5279 1425 -426 1769
 ATOM 1466 N GLY 210 23.951 7.786 59.869 1.000 25.89
 ANISOU 1466 N GLY 210 3802 2756 3278 523 899 749
 ATOM 1467 CA GLY 210 23.477 6.678 60.671 1.000 26.43
 ANISOU 1467 CA GLY 210 4479 2136 3427 1228 742 912
 ATOM 1468 C GLY 210 22.885 7.025 62.016 1.000 28.45
 ANISOU 1468 C GLY 210 5472 2099 3237 831 1029 1175
 ATOM 1469 O GLY 210 22.634 6.098 62.789 1.000 40.26
 ANISOU 1469 O GLY 210 7322 2719 5256 1881 2759 2360
 ATOM 1470 N ALA 211 22.651 8.281 62.338 1.000 25.78
 ANISOU 1470 N ALA 211 4671 2359 2763 1370 724 1197
 ATOM 1471 CA ALA 211 22.048 8.671 63.613 1.000 23.74
 ANISOU 1471 CA ALA 211 2966 3156 2896 727 339 663
 ATOM 1472 CB ALA 211 23.093 9.333 64.496 1.000 29.57
 ANISOU 1472 CB ALA 211 2957 4372 3906 834 -96 69
 ATOM 1473 C ALA 211 20.900 9.626 63.360 1.000 21.19
 ANISOU 1473 C ALA 211 3090 2611 2350 484 178 741
 ATOM 1474 O ALA 211 20.936 10.381 62.399 1.000 23.91
 ANISOU 1474 O ALA 211 3771 2659 2653 -30 -66 930
 ATOM 1475 N PHE 212 19.889 9.629 64.204 1.000 19.88
 ANISOU 1475 N PHE 212 2603 2577 2375 398 -128 374
 ATOM 1476 CA PHE 212 18.814 10.613 64.130 1.000 19.13
 ANISOU 1476 CA PHE 212 2581 2257 2432 284 -565 317
 ATOM 1477 C PHE 212 19.320 12.006 64.489 1.000 20.00
 ANISOU 1477 C PHE 212 3004 2480 2115 133 -640 68
 ATOM 1478 O PHE 212 19.893 12.230 65.569 1.000 21.10
 ANISOU 1478 O PHE 212 2497 3558 1964 -391 -406 222
 ATOM 1479 CB PHE 212 17.688 10.290 65.096 1.000 21.37
 ANISOU 1479 CB PHE 212 2553 2616 2952 293 -197 -184
 ATOM 1480 CG PHE 212 17.010 8.950 64.912 1.000 23.45
 ANISOU 1480 CG PHE 212 2161 3496 3253 -376 -282 -558
 ATOM 1481 CD1 PHE 212 16.369 8.377 65.990 1.000 23.33
 ANISOU 1481 CD1 PHE 212 2545 3115 3206 -382 -350 -508
 ATOM 1482 CD2 PHE 212 17.029 8.302 63.687 1.000 25.83
 ANISOU 1482 CD2 PHE 212 2554 3962 3299 -622 -217 -787
 ATOM 1483 CE1 PHE 212 15.730 7.149 65.872 1.000 28.13
 ANISOU 1483 CE1 PHE 212 3784 3544 3362 -1119 96 -973
 ATOM 1484 CE2 PHE 212 16.419 7.072 63.569 1.000 23.04
 ANISOU 1484 CE2 PHE 212 2504 2960 3289 382 -232 -558
 ATOM 1485 CZ PHE 212 15.781 6.486 64.651 1.000 27.88
 ANISOU 1485 CZ PHE 212 3658 3977 2957 -1072 -501 -760
 ATOM 1486 N THR 213 19.076 12.936 63.578 1.000 18.30
 ANISOU 1486 N THR 213 2690 2083 2181 149 -583 -93
 ATOM 1487 CA THR 213 19.566 14.310 63.681 1.000 17.99
 ANISOU 1487 CA THR 213 1976 2139 2721 230 -686 -287
 ATOM 1488 CB THR 213 20.515 14.586 62.498 1.000 20.43
 ANISOU 1488 CB THR 213 1798 2280 3683 140 -119 -423
 ATOM 1489 OG1 THR 213 21.638 13.695 62.629 1.000 25.33
 ANISOU 1489 OG1 THR 213 2571 3378 3676 925 71 528
 ATOM 1490 CG2 THR 213 21.087 15.985 62.485 1.000 21.11
 ANISOU 1490 CG2 THR 213 1935 2667 3420 -310 -289 -747
 ATOM 1491 C THR 213 18.391 15.277 63.641 1.000 15.53
 ANISOU 1491 C THR 213 1732 2135 2032 111 -557 -167
 ATOM 1492 O THR 213 17.533 15.195 62.761 1.000 16.11
 ANISOU 1492 O THR 213 1742 2197 2180 -327 -669 56
 ATOM 1493 N ASP 214 18.362 16.199 64.590 1.000 15.60
 ANISOU 1493 N ASP 214 2025 2046 1857 64 -405 2
 ATOM 1494 CA ASP 214 17.380 17.256 64.672 1.000 15.59
 ANISOU 1494 CA ASP 214 2130 1722 2072 2 -1010 -242
 ATOM 1495 CB ASP 214 17.744 18.200 65.822 1.000 17.13

- 139 -

ANISOU 1495 CB ASP 214 2528 1893 2086 -226 -1022 -247
 ATOM 1496 CG ASP 214 17.612 17.672 67.219 1.000 20.21
 ANISOU 1496 CG ASP 214 3138 2495 2045 -451 -1276 -148
 ATOM 1497 OD1 ASP 214 17.079 16.571 67.460 1.000 20.87
 ANISOU 1497 OD1 ASP 214 2778 2632 2518 -247 -505 151
 ATOM 1498 OD2 ASP 214 18.076 18.401 68.127 1.000 28.05
 ANISOU 1498 OD2 ASP 214 5110 3118 2429 -257 -1997 -619
 ATOM 1499 C ASP 214 17.314 18.146 63.441 1.000 15.14
 ANISOU 1499 C ASP 214 2029 1822 1901 182 -574 -319
 ATOM 1500 O ASP 214 18.349 18.552 62.897 1.000 17.63
 ANISOU 1500 O ASP 214 1956 2032 2710 -214 -810 -15
 ATOM 1501 N LEU 215 16.105 18.493 63.027 1.000 14.69
 ANISOU 1501 N LEU 215 1936 1758 1887 38 -334 242
 ATOM 1502 CA LEU 215 15.915 19.504 61.979 1.000 13.35
 ANISOU 1502 CA LEU 215 1820 1753 1498 89 -22 59
 ATOM 1503 CB LEU 215 15.352 18.819 60.734 1.000 14.24
 ANISOU 1503 CB LEU 215 1735 2167 1506 -98 75 -3
 ATOM 1504 CG LEU 215 16.291 17.813 60.056 1.000 16.39
 ANISOU 1504 CG LEU 215 2031 2285 1911 -340 320 -424
 ATOM 1505 CD1 LEU 215 15.517 16.999 59.031 1.000 22.61
 ANISOU 1505 CD1 LEU 215 3139 2024 3427 -10 -801 -877
 ATOM 1506 CD2 LEU 215 17.482 18.543 59.434 1.000 26.93
 ANISOU 1506 CD2 LEU 215 1998 5409 2827 -1083 909 -542
 ATOM 1507 C LEU 215 15.002 20.622 62.500 1.000 14.65
 ANISOU 1507 C LEU 215 1770 1607 2190 86 -165 -95
 ATOM 1508 O LEU 215 13.822 20.662 62.151 1.000 19.45
 ANISOU 1508 O LEU 215 1748 2165 3476 116 -303 -203
 ATOM 1509 N PRO 216 15.552 21.523 63.314 1.000 15.99
 ANISOU 1509 N PRO 216 2390 1970 1715 -164 21 -175
 ATOM 1510 CD PRO 216 16.955 21.601 63.757 1.000 19.37
 ANISOU 1510 CD PRO 216 2900 2306 2155 -83 -790 -548
 ATOM 1511 CA PRO 216 14.760 22.620 63.846 1.000 18.68
 ANISOU 1511 CA PRO 216 3104 2017 1976 12 -74 -420
 ATOM 1512 CB PRO 216 15.649 23.227 64.949 1.000 18.63
 ANISOU 1512 CB PRO 216 3592 1517 1971 -120 -421 9
 ATOM 1513 CG PRO 216 17.030 22.847 64.581 1.000 22.35
 ANISOU 1513 CG PRO 216 3401 2426 2666 -419 -427 -783
 ATOM 1514 C PRO 216 14.461 23.700 62.819 1.000 18.50
 ANISOU 1514 C PRO 216 2921 2083 2026 58 -465 -473
 ATOM 1515 O PRO 216 15.024 23.854 61.731 1.000 19.82
 ANISOU 1515 O PRO 216 2752 2453 2325 -32 -375 19
 ATOM 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
 ANISOU 1516 N TYR 217 3213 1981 2422 90 -482 -718
 ATOM 1517 CA TYR 217 13.178 25.662 62.308 1.000 22.97
 ANISOU 1517 CA TYR 217 2849 2652 3227 211 -1467 -313
 ATOM 1518 C TYR 217 14.347 26.647 62.283 1.000 23.92
 ANISOU 1518 C TYR 217 4139 2131 2819 -337 -1776 -165
 ATOM 1519 O TYR 217 15.149 26.726 63.213 1.000 30.46
 ANISOU 1519 O TYR 217 4321 3440 3812 -1118 -2477 728
 ATOM 1520 CB TYR 217 11.891 26.314 62.768 1.000 32.68
 ANISOU 1520 CB TYR 217 3958 3294 5164 1148 -874 -783
 ATOM 1521 CG TYR 217 12.064 27.462 63.718 1.000 44.77
 ANISOU 1521 CG TYR 217 6829 4326 5854 895 38 -1870
 ATOM 1522 CD1 TYR 217 11.853 28.763 63.285 1.000 54.26
 ANISOU 1522 CD1 TYR 217 10311 3688 6615 -323 132 -1945
 ATOM 1523 CD2 TYR 217 12.428 27.243 65.043 1.000 57.77
 ANISOU 1523 CD2 TYR 217 10635 5155 6158 -1027 -1446 -1931
 ATOM 1524 CE1 TYR 217 12.011 29.816 64.174 1.000 60.33
 ANISOU 1524 CE1 TYR 217 11807 4345 6772 -1101 -132 -2259
 ATOM 1525 CE2 TYR 217 12.585 28.296 65.926 1.000 64.51
 ANISOU 1525 CE2 TYR 217 12481 5199 6832 -1936 -1520 -2074

- 140 -

ATOM	1526	CZ	TYR	217	12.378	29.586	65.481	1.000	64.11	
ANISOU	1526	CZ	TYR	217	12047	5183	7129	-1460	-817	-2160
ATOM	1527	OH	TYR	217	12.536	30.639	66.358	1.000	63.69	
ANISOU	1527	OH	TYR	217	11840	5206	7153	-1832	-1191	-2064
ATOM	1528	N	ARG	218	14.418	27.374	61.188	1.000	24.08	
ANISOU	1528	N	ARG	218	4482	1611	3055	507	-1471	-145
ATOM	1529	CA	ARG	218	15.335	28.465	60.948	1.000	30.71	
ANISOU	1529	CA	ARG	218	5932	2490	3245	-504	-1565	382
ATOM	1530	CB	ARG	218	16.326	28.135	59.840	1.000	35.08	
ANISOU	1530	CB	ARG	218	5969	2797	4562	-1397	-779	-348
ATOM	1531	CG	ARG	218	17.401	27.114	60.073	1.000	35.77	
ANISOU	1531	CG	ARG	218	6009	3087	4497	-1107	-733	-773
ATOM	1532	CD	ARG	218	18.658	27.775	60.626	1.000	34.46	
ANISOU	1532	CD	ARG	218	5680	3264	4152	-1242	-244	-619
ATOM	1533	NE	ARG	218	19.223	28.746	59.709	1.000	29.51	
ANISOU	1533	NE	ARG	218	4707	2579	3926	7881	-629	
ATOM	1534	CZ	ARG	218	20.218	28.620	58.830	1.000	33.18	
ANISOU	1534	CZ	ARG	218	5269	3166	4170	60452	-1075	
ATOM	1535	NH1	ARG	218	20.839	27.452	58.709	1.000	27.44	
ANISOU	1535	NH1	ARG	218	4202	2881	3341	-503	-373	-1585
ATOM	1536	NH2	ARG	218	20.583	29.675	58.077	1.000	22.96	
ANISOU	1536	NH2	ARG	218	2327	3579	2817	233	-1117	-872
ATOM	1537	C	ARG	218	14.513	29.655	60.464	1.000	31.05	
ANISOU	1537	C	ARG	218	7353	1949	2496	-448	-1823	197
ATOM	1538	O	ARG	218	14.114	29.533	59.295	1.000	40.40	
ANISOU	1538	O	ARG	218	9873	2241	3235	531	-3168	-627
ATOM	1539	N	PRO	219	14.246	30.747	61.157	1.000	30.01	
ANISOU	1539	N	PRO	219	6290	2559	2555	-499	-1839	-284
ATOM	1540	CD	PRO	219	14.597	31.043	62.543	1.000	36.79	
ANISOU	1540	CD	PRO	219	8147	2878	2954	-1848	-2548	-374
ATOM	1541	CA	PRO	219	13.464	31.841	60.549	1.000	26.34	
ANISOU	1541	CA	PRO	219	4421	2564	3025	-573	-988	-340
ATOM	1542	CB	PRO	219	13.523	32.993	61.563	1.000	32.44	
ANISOU	1542	CB	PRO	219	5361	2891	4073	-691	-417	-989
ATOM	1543	CG	PRO	219	13.947	32.372	62.825	1.000	38.75	
ANISOU	1543	CG	PRO	219	7916	3462	3344	-1981	-958	-1235
ATOM	1544	C	PRO	219	14.005	32.329	59.220	1.000	23.64	
ANISOU	1544	C	PRO	219	3472	2066	3443	-161	-1028	109
ATOM	1545	O	PRO	219	13.300	32.950	58.412	1.000	30.61	
ANISOU	1545	O	PRO	219	4358	2934	4339	-347	-1712	876
ATOM	1546	N	ASP	220	15.269	32.087	58.906	1.000	25.98	
ANISOU	1546	N	ASP	220	3611	1756	4506	-389	-644	-815
ATOM	1547	CA	ASP	220	15.847	32.660	57.705	1.000	27.96	
ANISOU	1547	CA	ASP	220	3951	1603	5071	-364	30	-824
ATOM	1548	CB	ASP	220	17.212	33.238	58.155	1.000	29.61	
ANISOU	1548	CB	ASP	220	3549	3142	4558	-176	-326	176
ATOM	1549	CG	ASP	220	18.091	32.158	58.780	1.000	32.09	
ANISOU	1549	CG	ASP	220	3706	3527	4961	625	978	615
ATOM	1550	OD1	ASP	220	17.697	31.434	59.719	1.000	26.12	
ANISOU	1550	OD1	ASP	220	3013	3522	3390	-158	-289	-97
ATOM	1551	OD2	ASP	220	19.241	32.088	58.281	1.000	29.09	
ANISOU	1551	OD2	ASP	220	3714	3756	3581	304	677	-712
ATOM	1552	C	ASP	220	16.037	31.726	56.525	1.000	25.26	
ANISOU	1552	C	ASP	220	2508	1291	5800	354	1110	-822
ATOM	1553	O	ASP	220	16.641	32.095	55.515	1.000	28.28	
ANISOU	1553	O	ASP	220	4088	1665	4994	-855	298	-434
ATOM	1554	N	ALA	221	15.500	30.510	56.631	1.000	21.58	
ANISOU	1554	N	ALA	221	2748	1770	3681	-288	178	-651
ATOM	1555	CA	ALA	221	15.840	29.484	55.658	1.000	19.81	
ANISOU	1555	CA	ALA	221	2986	1452	3090	-342	-224	-315
ATOM	1556	CB	ALA	221	17.130	28.800	56.109	1.000	19.51	

- 141 -

ANISOU	1556	CB	ALA	221	2267	1497	3647	-648	45	-746
ATOM	1557	C	ALA	221	14.718	28.469	55.489	1.000	17.71	
ANISOU	1557	C	ALA	221	2304	1912	2512	-251	-75	-309
ATOM	1558	O	ALA	221	13.866	28.356	56.380	1.000	20.97	
ANISOU	1558	O	ALA	221	3596	2029	2344	-503	406	-284
ATOM	1559	N	VAL	222	14.728	27.756	54.378	1.000	14.22	
ANISOU	1559	N	VAL	222	1560	1582	2262	-76	-92	-11
ATOM	1560	CA	VAL	222	13.823	26.617	54.160	1.000	14.89	
ANISOU	1560	CA	VAL	222	1326	1608	2723	98	-216	-205
ATOM	1561	CB	VAL	222	13.079	26.779	52.830	1.000	17.28	
ANISOU	1561	CB	VAL	222	1680	1754	3133	90	-657	-144
ATOM	1562	CG1	VAL	222	13.995	26.685	51.620	1.000	19.17	
ANISOU	1562	CG1	VAL	222	1974	2625	2686	-446	-775	150
ATOM	1563	CG2	VAL	222	11.996	25.747	52.641	1.000	17.36	
ANISOU	1563	CG2	VAL	222	2185	1879	2533	-254	-362	-385
ATOM	1564	C	VAL	222	14.653	25.339	54.263	1.000	12.66	
ANISOU	1564	C	VAL	222	1136	1564	2112	-50	-225	-378
ATOM	1565	O	VAL	222	15.828	25.320	53.893	1.000	13.12	
ANISOU	1565	O	VAL	222	1280	1825	1881	104	-13	-199
ATOM	1566	N	LEU	223	14.049	24.267	54.775	1.000	12.98	
ANISOU	1566	N	LEU	223	1123	1538	2270	-163	-370	-417
ATOM	1567	CA	LEU	223	14.681	22.952	54.749	1.000	10.70	
ANISOU	1567	CA	LEU	223	891 1704	1472	-26	-98	-7	
ATOM	1568	CB	LEU	223	14.276	22.130	55.961	1.000	13.02	
ANISOU	1568	CB	LEU	223	1387	1968	1593	-419	289	-108
ATOM	1569	CG	LEU	223	14.739	20.683	56.106	1.000	17.41	
ANISOU	1569	CG	LEU	223	2434	2132	2050	-290	-476	566
ATOM	1570	CD1	LEU	223	16.247	20.614	56.204	1.000	17.20	
ANISOU	1570	CD1	LEU	223	2576	1518	2441	26	-989	-249
ATOM	1571	CD2	LEU	223	13.983	20.076	57.282	1.000	33.63	
ANISOU	1571	CD2	LEU	223	3981	4721	4077	-341	134	2949
ATOM	1572	C	LEU	223	14.362	22.211	53.456	1.000	10.02	
ANISOU	1572	C	LEU	223	1000	1265	1543	58	-319	88
ATOM	1573	O	LEU	223	13.206	22.160	53.088	1.000	12.86	
ANISOU	1573	O	LEU	223	949 1945	1992	-97	-174	-372	
ATOM	1574	N	VAL	224	15.406	21.675	52.798	1.000	10.55	
ANISOU	1574	N	VAL	224	978 1070	1962	-76	-418	-382	
ATOM	1575	CA	VAL	224	15.227	20.932	51.553	1.000	11.98	
ANISOU	1575	CA	VAL	224	1376	1288	1887	-249	-278	-372
ATOM	1576	CB	VAL	224	16.095	21.461	50.391	1.000	11.23	
ANISOU	1576	CB	VAL	224	901 1541	1824	-279	-622	-99	
ATOM	1577	CG1	VAL	224	15.833	20.690	49.102	1.000	13.16	
ANISOU	1577	CG1	VAL	224	1899	1485	1615	-462	-516	84
ATOM	1578	CG2	VAL	224	15.837	22.941	50.156	1.000	13.86	
ANISOU	1578	CG2	VAL	224	1480	1520	2266	-135	-354	-64
ATOM	1579	C	VAL	224	15.539	19.450	51.786	1.000	10.87	
ANISOU	1579	C	VAL	224	953 1275	1901	-13	342	-484	
ATOM	1580	O	VAL	224	16.646	19.148	52.201	1.000	12.57	
ANISOU	1580	O	VAL	224	1283	1363	2132	-175	-154	-274
ATOM	1581	N	PHE	225	14.585	18.553	51.533	1.000	11.86	
ANISOU	1581	N	PHE	225	1241	1128	2137	-15	-303	-61
ATOM	1582	CA	PHE	225	14.811	17.130	51.412	1.000	11.38	
ANISOU	1582	CA	PHE	225	1260	1157	1909	-22	-67	-56
ATOM	1583	CB	PHE	225	13.707	16.280	52.044	1.000	11.34	
ANISOU	1583	CB	PHE	225	1117	1176	2015	205	-213	335
ATOM	1584	CG	PHE	225	13.654	16.172	53.544	1.000	11.38	
ANISOU	1584	CG	PHE	225	964 1369	1991	-251	-333	181	
ATOM	1585	CD1	PHE	225	14.685	15.653	54.291	1.000	15.28	
ANISOU	1585	CD1	PHE	225	1771	1777	2256	-98	-853	298
ATOM	1586	CD2	PHE	225	12.532	16.576	54.254	1.000	17.91	
ANISOU	1586	CD2	PHE	225	1904	2748	2153	341	106	0

- 142 -

ATOM	1587	CE1	PHE	225	14.619	15.535	55.661	1.000	17.46	
ANISOU	1587	CE1	PHE	225	2449	1862	2321	-249	-795	6 6 6
ATOM	1588	CE2	PHE	225	12.447	16.474	55.612	1.000	19.35	
ANISOU	1588	CE2	PHE	225	2563	2678	2111	121	129	- 1 1
ATOM	1589	CZ	PHE	225	13.499	15.945	56.341	1.000	18.20	
ANISOU	1589	CZ	PHE	225	2952	1641	2324	-501	-470	3 6
ATOM	1590	C	PHE	225	14.907	16.774	49.927	1.000	12.03	
ANISOU	1590	C	PHE	225	1480	1285	1804	130	-201	4 2
ATOM	1591	O	PHE	225	14.019	17.160	49.163	1.000	12.77	
ANISOU	1591	O	PHE	225	1473	1466	1912	341	-118	3 8
ATOM	1592	N	CYS	226	15.940	16.032	49.521	1.000	9.62	
ANISOU	1592	N	CYS	226	954 1403	1296	-204	-407	2 9	
ATOM	1593	CA	CYS	226	15.917	15.400	48.197	1.000	10.80	
ANISOU	1593	CA	CYS	226	1432	1204	1468	-258	-310	- 5 9
ATOM	1594	CB	CYS	226	17.337	15.029	47.744	1.000	12.02	
ANISOU	1594	CB	CYS	226	1539	1362	1666	-357	16	- 12 5
ATOM	1595	SG	CYS	226	18.426	16.490	47.554	1.000	13.74	
ANISOU	1595	SG	CYS	226	1627	1400	2192	-341	18	1 3 9
ATOM	1596	C	CYS	226	14.998	14.178	48.256	1.000	9.86	
ANISOU	1596	C	CYS	226	1190	1061	1495	-20	-293	- 1 6
ATOM	1597	O	CYS	226	15.015	13.431	49.252	1.000	11.17	
ANISOU	1597	O	CYS	226	1181	1280	1781	-129	-435	2 7 2
ATOM	1598	N	GLY	227	14.217	13.963	47.205	1.000	10.17	
ANISOU	1598	N	GLY	227	1428	1010	1427	-258	-271	- 3 5
ATOM	1599	CA	GLY	227	13.370	12.806	47.053	1.000	9.73	
ANISOU	1599	CA	GLY	227	1231	860 1604	-178	-74	- 3 7	
ATOM	1600	C	GLY	227	13.908	11.769	46.074	1.000	9.48	
ANISOU	1600	C	GLY	227	1438	717 1445	16	-35	1 6 9	
ATOM	1601	O	GLY	227	14.935	11.961	45.402	1.000	9.86	
ANISOU	1601	O	GLY	227	1321	1137	1290	-104	-179	7 8
ATOM	1602	N	ALA	228	13.217	10.631	45.971	1.000	9.17	
ANISOU	1602	N	ALA	228	1279	729 1477	109	-135	5 8	
ATOM	1603	CA	ALA	228	13.650	9.529	45.108	1.000	9.41	
ANISOU	1603	CA	ALA	228	1315	887 1371	9	-74	- 5 2	
ATOM	1604	CB	ALA	228	12.727	8.296	45.256	1.000	10.50	
ANISOU	1604	CB	ALA	228	2011	824 1155	-143	124	1 0 1	
ATOM	1605	C	ALA	228	13.712	9.918	43.637	1.000	9.25	
ANISOU	1605	C	ALA	228	1343	666 1507	-108	90	1 3 9	
ATOM	1606	O	ALA	228	14.493	9.305	42.895	1.000	9.48	
ANISOU	1606	O	ALA	228	1171	1026	1405	-88	-50	9 0
ATOM	1607	N	ILE	229	12.970	10.907	43.143	1.000	10.30	
ANISOU	1607	N	ILE	229	1402	1004	1509	18	25	1 7 7
ATOM	1608	CA	ILE	229	13.074	11.311	41.727	1.000	10.87	
ANISOU	1608	CA	ILE	229	1197	1446	1487	-2	-159	2 5 1
ATOM	1609	CB	ILE	229	11.802	12.078	41.295	1.000	11.52	
ANISOU	1609	CB	ILE	229	1257	1473	1647	34	-57	3 6 2
ATOM	1610	CG2	ILE	229	11.997	12.852	39.999	1.000	11.30	
ANISOU	1610	CG2	ILE	229	1655	1211	1426	83	-189	1 5 6
ATOM	1611	CG1	ILE	229	10.575	11.131	41.237	1.000	14.39	
ANISOU	1611	CG1	ILE	229	1031	2034	2402	-40	210	3 1 1
ATOM	1612	CD1	ILE	229	10.676	10.093	40.138	1.000	19.20	
ANISOU	1612	CD1	ILE	229	2085	1723	3489	-610	93	- 13 8
ATOM	1613	C	ILE	229	14.389	12.034	41.477	1.000	10.38	
ANISOU	1613	C	ILE	229	1293	1405	1247	-62	-169	3 2 2
ATOM	1614	O	ILE	229	14.952	11.947	40.369	1.000	11.66	
ANISOU	1614	O	ILE	229	1805	1257	1368	-13	145	3 2 8
ATOM	1615	N	ALA	230	14.965	12.692	42.490	1.000	10.66	
ANISOU	1615	N	ALA	230	1476	1274	1300	-104	-151	3 5 6
ATOM	1616	CA	ALA	230	16.312	13.259	42.338	1.000	11.21	
ANISOU	1616	CA	ALA	230	1473	975 1813	-57	-308	9 0	
ATOM	1617	CB	ALA	230	16.681	14.148	43.509	1.000	10.58	

- 143 -

ANISOU	1617	CB	ALA	230	1350	1295	1375	62	-106	1	2	6
ATOM	1618	C	ALA	230	17.336	12.136	42.132	1.000	11	2	8	
ANISOU	1618	C	ALA	230	1640	1037	1610	1	55	2	4	2
ATOM	1619	O	ALA	230	18.220	12.185	41.273	1.000	11	2	9	
ANISOU	1619	O	ALA	230	1510	1240	1539	-189	-40	2	8	8
ATOM	1620	N	THR	231	17.173	11.097	42.946	1.000	10	5	5	
ANISOU	1620	N	THR	231	1328	894	1787	-262	-70	2	1	4
ATOM	1621	CA	THR	231	18.064	9.939	42.819	1.000	11	9	8	
ANISOU	1621	CA	THR	231	1929	1018	1605	0	-164	1	5	9
ATOM	1622	CB	THR	231	17.717	8.865	43.878	1.000	10	7	6	
ANISOU	1622	CB	THR	231	1381	1070	1636	-86	-453	2	4	6
ATOM	1623	OG1	THR	231	17.658	9.437	45.198	1.000	11	8	2	
ANISOU	1623	OG1	THR	231	1615	1236	1641	35	-115	2	7	7
ATOM	1624	CG2	THR	231	18.765	7.752	43.880	1.000	12	5	7	
ANISOU	1624	CG2	THR	231	1621	1314	1840	160	-89	3	5	1
ATOM	1625	C	THR	231	17.958	9.352	41.415	1.000	12	5	2	
ANISOU	1625	C	THR	231	1632	1500	1624	-145	42	1	1	
ATOM	1626	O	THR	231	18.939	9.050	40.732	1.000	12	1	5	
ANISOU	1626	O	THR	231	1636	1233	1747	-17	86	2	2	4
ATOM	1627	N	LEU	232	16.717	9.154	40.959	1.000	11	1	4	
ANISOU	1627	N	LEU	232	1608	1005	1620	90	-68	1	4	1
ATOM	1628	CA	LEU	232	16.446	8.522	39.675	1.000	12	4	7	
ANISOU	1628	CA	LEU	232	1880	1203	1657	109	-169	4	5	
ATOM	1629	CB	LEU	232	14.950	8.214	39.552	1.000	12	8	1	
ANISOU	1629	CB	LEU	232	1989	1225	1654	-78	-209	1	9	
ATOM	1630	CG	LEU	232	14.452	7.464	38.314	1.000	14	8	5	
ANISOU	1630	CG	LEU	232	2171	1753	1719	-5	-410	-	9	6
ATOM	1631	CD1	LEU	232	15.020	6.055	38.240	1.000	16	7	8	
ANISOU	1631	CD1	LEU	232	2693	1749	1932	72	-431	-	4	8
ATOM	1632	CD2	LEU	232	12.914	7.411	38.291	1.000	15	7	0	
ANISOU	1632	CD2	LEU	232	2180	1866	1920	-278	-589	4	9	4
ATOM	1633	C	LEU	232	16.964	9.354	38.511	1.000	11	5	8	
ANISOU	1633	C	LEU	232	1452	1390	1559	309	-301	1	3	6
ATOM	1634	O	LEU	232	17.752	8.837	37.686	1.000	13	4	5	
ANISOU	1634	O	LEU	232	1808	1436	1867	320	-17	3	0	
ATOM	1635	N	VAL	233	16.565	10.617	38.414	1.000	10	9	5	
ANISOU	1635	N	VAL	233	1428	1210	1522	-14	-210	0		
ATOM	1636	CA	VAL	233	16.948	11.421	37.242	1.000	11	7	0	
ANISOU	1636	CA	VAL	233	1703	1345	1397	97	5	1	3	
ATOM	1637	CB	VAL	233	16.156	12.743	37.215	1.000	11	1	4	
ANISOU	1637	CB	VAL	233	1672	1272	1287	-26	276	7	3	
ATOM	1638	CG1	VAL	233	16.661	13.774	38.249	1.000	13	3	4	
ANISOU	1638	CG1	VAL	233	1834	1562	1673	-205	653	-	3	6
ATOM	1639	CG2	VAL	233	16.106	13.412	35.827	1.000	14	6	6	
ANISOU	1639	CG2	VAL	233	1992	1873	1704	-4	-45	5	8	6
ATOM	1640	C	VAL	233	18.459	11.586	37.132	1.000	13	4	1	
ANISOU	1640	C	VAL	233	1712	1573	1811	91	151	1	2	5
ATOM	1641	O	VAL	233	19.012	11.627	36.021	1.000	13	4	5	
ANISOU	1641	O	VAL	233	1844	1402	1866	46	192	4	3	8
ATOM	1642	N	THR	234	19.188	11.665	38.250	1.000	13	1	3	
ANISOU	1642	N	THR	234	1457	1639	1893	-139	223	1	2	6
ATOM	1643	CA	THR	234	20.613	11.930	38.244	1.000	13	0	0	
ANISOU	1643	CA	THR	234	1483	1600	1855	-188	428	1	4	3
ATOM	1644	CB	THR	234	21.069	12.726	39.465	1.000	12	4	6	
ANISOU	1644	CB	THR	234	1300	1632	1803	-32	200	2	5	1
ATOM	1645	OG1	THR	234	20.825	11.941	40.639	1.000	13	7	1	
ANISOU	1645	OG1	THR	234	1660	1662	1888	192	202	2	9	1
ATOM	1646	CG2	THR	234	20.301	14.027	39.643	1.000	11	3	7	
ANISOU	1646	CG2	THR	234	1097	1565	1657	-153	-87	1	6	9
ATOM	1647	C	THR	234	21.424	10.643	38.178	1.000	14	4	4	
ANISOU	1647	C	THR	234	1550	1823	2114	6	-73	-	5	3

- 144 -

ATOM	1648	O	THR	234	22.659	10.710	38.233	1.000	15.81
ANISOU	1648	O	THR	234	1546	2169	2293	61 27	2 1 7
ATOM	1649	N	GLY	235	20.767	9.477	38.070	1.000	14.76
ANISOU	1649	N	GLY	235	1776	1576	2254	77 81	4 1 0
ATOM	1650	CA	GLY	235	21.530	8.249	37.994	1.000	16.69
ANISOU	1650	CA	GLY	235	2053	1803	2486	304	35 1 8 9
ATOM	1651	C	GLY	235	22.243	7.862	39.275	1.000	16.83
ANISOU	1651	C	GLY	235	1854	2031	2512	765	244 1 9 3
ATOM	1652	O	GLY	235	23.305	7.237	39.194	1.000	19.67
ANISOU	1652	O	GLY	235	2074	2172	3225	1035	383 3 7 2
ATOM	1653	N	GLY	236	21.665	8.227	40.425	1.000	14.46
ANISOU	1653	N	GLY	236	1732	1327	2433	154	198 7 5
ATOM	1654	CA	GLY	236	22.187	7.768	41.692	1.000	15.73
ANISOU	1654	CA	GLY	236	2060	1381	2536	41 186	3 1 2
ATOM	1655	C	GLY	236	23.166	8.691	42.388	1.000	14.76
ANISOU	1655	C	GLY	236	1931	1332	2346	252	73 2 8 8
ATOM	1656	O	GLY	236	23.778	8.244	43.373	1.000	18.32
ANISOU	1656	O	GLY	236	1983	2197	2782	106	-105 8 4 4
ATOM	1657	N	GLN	237	23.318	9.938	41.953	1.000	13.99
ANISOU	1657	N	GLN	237	1831	1349	2137	158	165 1 7 0
ATOM	1658	CA	GLN	237	24.209	10.956	42.485	1.000	13.13
ANISOU	1658	CA	GLN	237	1474	1304	2210	367	-31 2 7 6
ATOM	1659	CB	GLN	237	24.629	11.948	41.383	1.000	13.38
ANISOU	1659	CB	GLN	237	1367	1566	2151	99 72	1 5 9
ATOM	1660	CG	GLN	237	25.390	11.335	40.219	1.000	14.74
ANISOU	1660	CG	GLN	237	1404	1529	2666	518	410 3 3 3
ATOM	1661	CD	GLN	237	25.816	12.428	39.257	1.000	17.22
ANISOU	1661	CD	GLN	237	2039	2018	2486	-64	426 3 6 0
ATOM	1662	OE1	GLN	237	26.754	13.208	39.522	1.000	20.60
ANISOU	1662	OE1	GLN	237	1566	2334	3928	-10	-29 9 6 5
ATOM	1663	NE2	GLN	237	25.116	12.470	38.127	1.000	17.47
ANISOU	1663	NE2	GLN	237	2014	2093	2533	208	438 4 0 8
ATOM	1664	C	GLN	237	23.627	11.739	43.663	1.000	12.90
ANISOU	1664	C	GLN	237	1474	1324	2104	72 -10	2 5 5
ATOM	1665	O	GLN	237	24.332	12.549	44.282	1.000	15.90
ANISOU	1665	O	GLN	237	1739	1888	2413	-291	74 - 8 4
ATOM	1666	N	VAL	238	22.365	11.481	44.013	1.000	12.13
ANISOU	1666	N	VAL	238	1372	962 2276	212	-33	2 0 0
ATOM	1667	CA	VAL	238	21.664	12.182	45.082	1.000	11.91
ANISOU	1667	CA	VAL	238	1169	1436	1920	-121	-276 - 1 9
ATOM	1668	CB	VAL	238	20.622	13.158	44.510	1.000	12.00
ANISOU	1668	CB	VAL	238	1024	1179	2357	-6 199	- 3 1
ATOM	1669	CG1	VAL	238	19.978	13.999	45.601	1.000	13.07
ANISOU	1669	CG1	VAL	238	1530	1668	1767	63 -232	- 2 2 2
ATOM	1670	CG2	VAL	238	21.207	14.088	43.463	1.000	14.00
ANISOU	1670	CG2	VAL	238	1795	1470	2053	-40	- 2 1 8 1
ATOM	1671	C	VAL	238	20.990	11.156	46.000	1.000	13.62
ANISOU	1671	C	VAL	238	1707	1415	2054	-103	-40 - 2 2
ATOM	1672	O	VAL	238	20.252	10.288	45.492	1.000	12.64
ANISOU	1672	O	VAL	238	1702	977 2123	60	-318	2 5 7
ATOM	1673	N	LYS	239	21.247	11.246	47.300	1.000	11.99
ANISOU	1673	N	LYS	239	1075	1404	2076	127	-101 7 4
ATOM	1674	CA	LYS	239	20.568	10.444	48.322	1.000	12.77
ANISOU	1674	CA	LYS	239	1224	1541	2088	-12	-124 8 6
ATOM	1675	CB	LYS	239	21.382	10.463	49.622	1.000	12.23
ANISOU	1675	CB	LYS	239	1333	1155	2158	183	-234 - 2 8
ATOM	1676	CG	LYS	239	20.953	9.626	50.793	1.000	13.85
ANISOU	1676	CG	LYS	239	1643	1689	1931	187	-52 - 8 9
ATOM	1677	CD	LYS	239	21.927	9.579	51.957	1.000	20.13
ANISOU	1677	CD	LYS	239	2893	1795	2961	10	-1185 5 8 8
ATOM	1678	CE	LYS	239	21.364	8.745	53.098	1.000	24.73

- 145 -

ANISOU	1678	CE	LYS	239	4065	2250	3080	-348	-1466	1 0 6 4
ATOM	1679	NZ	LYS	239	22.019	8.841	54.420	1.000	32.28	
ANISOU	1679	NZ	LYS	239	5658	4315	2293	1610	-930	-3 0 4
ATOM	1680	C	LYS	239	19.169	10.949	48.661	1.000	11.59	
ANISOU	1680	C	LYS	239	1207	1332	1866	-35	-82	6 4
ATOM	1681	O	LYS	239	18.976	12.191	48.708	1.000	12.32	
ANISOU	1681	O	LYS	239	1638	1294	1749	-2	-25	2 3 6
ATOM	1682	N	ALA	240	18.222	10.047	48.863	1.000	10.65	
ANISOU	1682	N	ALA	240	1248	1266	1534	-52	-185	- 8 8
ATOM	1683	CA	ALA	240	16.884	10.368	49.354	1.000	10.21	
ANISOU	1683	CA	ALA	240	1292	1057	1531	-195	-37	-1 0 9
ATOM	1684	CB	ALA	240	15.784	9.782	48.466	1.000	13.46	
ANISOU	1684	CB	ALA	240	1195	2378	1543	-232	20	-4 0 3
ATOM	1685	C	ALA	240	16.784	9.881	50.807	1.000	10.97	
ANISOU	1685	C	ALA	240	1308	1249	1611	-127	-142	4 9
ATOM	1686	O	ALA	240	16.595	8.664	51.059	1.000	13.02	
ANISOU	1686	O	ALA	240	2136	1242	1568	-243	28	- 7
ATOM	1687	N	PRO	241	16.967	10.783	51.782	1.000	11.13	
ANISOU	1687	N	PRO	241	1723	1041	1466	160	-49	1 3 8
ATOM	1688	CD	PRO	241	17.172	12.237	51.654	1.000	11.17	
ANISOU	1688	CD	PRO	241	1419	1204	1618	-180	-128	7 6
ATOM	1689	CA	PRO	241	17.043	10.340	53.166	1.000	11.96	
ANISOU	1689	CA	PRO	241	1597	1447	1499	-172	-32	1 9 3
ATOM	1690	CB	PRO	241	17.712	11.545	53.891	1.000	14.25	
ANISOU	1690	CB	PRO	241	1875	1837	1701	-531	-383	2 4 2
ATOM	1691	CG	PRO	241	17.286	12.724	53.069	1.000	13.61	
ANISOU	1691	CG	PRO	241	2015	1446	1709	-596	-465	- 2 2
ATOM	1692	C	PRO	241	15.708	10.072	53.861	1.000	12.35	
ANISOU	1692	C	PRO	241	1417	1610	1665	-175	-187	4 1 8
ATOM	1693	O	PRO	241	14.759	10.829	53.655	1.000	12.28	
ANISOU	1693	O	PRO	241	1359	1582	1723	-232	-468	8 1
ATOM	1694	N	ARG	242	15.700	9.033	54.711	1.000	12.75	
ANISOU	1694	N	ARG	242	1775	1407	1664	-170	76	2 5 0
ATOM	1695	CA	ARG	242	14.563	8.804	55.576	1.000	10.76	
ANISOU	1695	CA	ARG	242	1292	1417	1380	-207	-281	2 1 1
ATOM	1696	CB	ARG	242	14.614	7.405	56.223	1.000	15.02	
ANISOU	1696	CB	ARG	242	2419	1368	1918	-357	117	2 9 4
ATOM	1697	CG	ARG	242	14.115	6.342	55.230	1.000	17.85	
ANISOU	1697	CG	ARG	242	3373	1274	2135	9	-560	2 5 1
ATOM	1698	CD	ARG	242	14.254	4.934	55.763	1.000	19.42	
ANISOU	1698	CD	ARG	242	3148	1111	3120	506	503	1 1 6
ATOM	1699	NE	ARG	242	15.667	4.552	55.849	1.000	20.71	
ANISOU	1699	NE	ARG	242	3225	2107	2538	938	638	2 1 2
ATOM	1700	CZ	ARG	242	16.107	3.444	56.416	1.000	23.22	
ANISOU	1700	CZ	ARG	242	3198	2206	3417	307	-544	5 8 9
ATOM	1701	NH1	ARG	242	15.285	2.567	56.980	1.000	24.46	
ANISOU	1701	NH1	ARG	242	4097	2112	3083	307	387	1 9 5
ATOM	1702	NH2	ARG	242	17.416	3.184	56.438	1.000	25.41	
ANISOU	1702	NH2	ARG	242	3402	2332	3921	819	-267	4 0 3
ATOM	1703	C	ARG	242	14.477	9.834	56.704	1.000	11.95	
ANISOU	1703	C	ARG	242	1571	1463	1506	-248	-214	1 0 7
ATOM	1704	O	ARG	242	15.469	10.377	57.213	1.000	13.65	
ANISOU	1704	O	ARG	242	1708	1439	2040	-322	-401	- 3 8
ATOM	1705	N	HIS	243	13.252	10.085	57.118	1.000	11.60	
ANISOU	1705	N	HIS	243	1657	1410	1342	-311	-206	5
ATOM	1706	CA	HIS	243	12.942	11.056	58.158	1.000	11.49	
ANISOU	1706	CA	HIS	243	1855	1571	938	-306	-183	1 4 0
ATOM	1707	CB	HIS	243	12.968	12.462	57.546	1.000	11.22	
ANISOU	1707	CB	HIS	243	1432	1379	1453	-231	-221	3 9
ATOM	1708	CG	HIS	243	12.133	12.694	56.341	1.000	11.80	
ANISOU	1708	CG	HIS	243	1937	1171	1378	-31	-268	7 9

- 146 -

ATOM	1709	CD2	HIS	243	10.885	13.236	56.181	1.000	11.15
ANISOU	1709	CD2	HIS	243	1990	1106	1142	35	-344 1 4 1
ATOM	1710	ND1	HIS	243	12.538	12.345	55.086	1.000	12.29
ANISOU	1710	ND1	HIS	243	1670	1606	1395	-394	-91 8
ATOM	1711	CE1	HIS	243	11.599	12.653	54.209	1.000	12.59
ANISOU	1711	CE1	HIS	243	1686	1740	1357	-522	-202 -2 5 3
ATOM	1712	NE2	HIS	243	10.585	13.204	54.841	1.000	10.77
ANISOU	1712	NE2	HIS	243	1612	1307	1172	-616	-268 -3 6
ATOM	1713	C	HIS	243	11.605	10.737	58.812	1.000	12.49
ANISOU	1713	C	HIS	243	1869	1570	1308	-321	-53 7 3
ATOM	1714	O	HIS	243	10.807	9.949	58.271	1.000	12.26
ANISOU	1714	O	HIS	243	1756	1404	1497	-188	-115 4 7
ATOM	1715	N	HIS	244	11.352	11.319	59.983	1.000	12.16
ANISOU	1715	N	HIS	244	1464	1715	1442	-230	-112 -3 2
ATOM	1716	CA	HIS	244	10.138	11.043	60.758	1.000	12.02
ANISOU	1716	CA	HIS	244	1606	1809	1152	-599	-167 -2 4
ATOM	1717	CB	HIS	244	10.255	9.778	61.615	1.000	12.51
ANISOU	1717	CB	HIS	244	1655	1763	1334	-19	101 -4 7
ATOM	1718	CG	HIS	244	11.270	9.810	62.698	1.000	15.04
ANISOU	1718	CG	HIS	244	2025	1723	1965	-178	-433 1 5 4
ATOM	1719	CD2	HIS	244	11.276	10.380	63.923	1.000	18.19
ANISOU	1719	CD2	HIS	244	2946	2339	1627	36	-732 2 9 7
ATOM	1720	ND1	HIS	244	12.504	9.203	62.662	1.000	19.30
ANISOU	1720	ND1	HIS	244	2303	2232	2800	229	-708 2 6 6
ATOM	1721	CE1	HIS	244	13.226	9.387	63.731	1.000	22.48
ANISOU	1721	CE1	HIS	244	2649	2734	3159	11	-1206 6 5 0
ATOM	1722	NE2	HIS	244	12.476	10.120	64.531	1.000	22.33
ANISOU	1722	NE2	HIS	244	3088	2895	2500	-272	-1236 3 8 4
ATOM	1723	C	HIS	244	9.780	12.246	61.613	1.000	13.47
ANISOU	1723	C	HIS	244	1897	1673	1549	-362	254 6 7
ATOM	1724	O	HIS	244	10.603	13.165	61.798	1.000	13.48
ANISOU	1724	O	HIS	244	1800	1726	1595	-283	139 -1 6 1
ATOM	1725	N	VAL	245	8.551	12.245	62.130	1.000	15.26
ANISOU	1725	N	VAL	245	1852	1964	1983	-417	232 -5 5
ATOM	1726	CA	VAL	245	8.090	13.352	62.970	1.000	17.31
ANISOU	1726	CA	VAL	245	2108	2442	2026	-125	476 -1 6 1
ATOM	1727	CB	VAL	245	6.939	14.169	62.360	1.000	17.33
ANISOU	1727	CB	VAL	245	2094	2473	2019	-80	340 -4 7 7
ATOM	1728	CG1	VAL	245	6.551	15.334	63.286	1.000	25.25
ANISOU	1728	CG1	VAL	245	2217	2966	4410	-137	1939 -1 2 4 8
ATOM	1729	CG2	VAL	245	7.252	14.713	60.966	1.000	21.49
ANISOU	1729	CG2	VAL	245	3070	2538	2556	-180	313 2 7 1
ATOM	1730	C	VAL	245	7.682	12.768	64.327	1.000	18.29
ANISOU	1730	C	VAL	245	2123	2689	2137	-443	508 -7 1
ATOM	1731	O	VAL	245	6.765	11.945	64.429	1.000	18.62
ANISOU	1731	O	VAL	245	1810	2174	3089	-15	451 2 5 4
ATOM	1732	N	ALA	246	8.385	13.202	65.369	1.000	21.54
ANISOU	1732	N	ALA	246	2813	3045	2327	-591	-407 9 0 7
ATOM	1733	CA	ALA	246	8.133	12.701	66.719	1.000	25.10
ANISOU	1733	CA	ALA	246	4596	2562	2379	94	-225 9 9 7
ATOM	1734	CB	ALA	246	9.424	12.723	67.537	1.000	29.82
ANISOU	1734	CB	ALA	246	5381	3408	2540	402	-889 1 3 2 5
ATOM	1735	C	ALA	246	7.080	13.545	67.412	1.000	31.20
ANISOU	1735	C	ALA	246	5079	4143	2632	314	280 4 2 8
ATOM	1736	O	ALA	246	6.876	14.714	67.052	1.000	32.39
ANISOU	1736	O	ALA	246	4706	3748	3853	567	1247 -6 6
ATOM	1737	N	ALA	247	6.429	12.973	68.413	1.000	37.30
ANISOU	1737	N	ALA	247	5548	5498	3126	92	640 8 3 5
ATOM	1738	CA	ALA	247	5.585	13.794	69.271	1.000	40.42
ANISOU	1738	CA	ALA	247	5434	6048	3878	15	1313 8 5 0
ATOM	1739	C	ALA	247	6.289	14.132	70.578	1.000	42.17

- 147 -

ANISOU	1739	C	ALA	247	6495	5891	3636	-823	1720	3	4	1
ATOM	1740	O	ALA	247	7.048	13.338	71.136	1.000	41.63			
ANISOU	1740	O	ALA	247	5811	6371	3637	-1631	804	4	2	5
ATOM	1741	CB	ALA	247	4.280	13.067	69.525	1.000	47.17			
ANISOU	1741	CB	ALA	247	5186	9059	3676	-520	523	2	6	8
ATOM	1742	N	SER	257	1.781	21.848	70.382	1.000	31.02			
ANISOU	1742	N	SER	257	4109	5558	2119	137	-235	-	8	1
ATOM	1743	CA	SER	257	1.214	21.932	69.052	1.000	27.01			
ANISOU	1743	CA	SER	257	2792	5165	2304	109	-143	-	7	0
ATOM	1744	CB	SER	257	0.039	22.914	68.992	1.000	28.16			
ANISOU	1744	CB	SER	257	2655	4473	3572	-238	-90	-	1	0
ATOM	1745	OG	SER	257	0.491	24.251	69.074	1.000	51.32			
ANISOU	1745	OG	SER	257	8516	4131	6853	-616	-2734	-	8	0
ATOM	1746	C	SER	257	2.259	22.389	68.034	1.000	26.19			
ANISOU	1746	C	SER	257	2537	5064	2350	-132	-413	-	5	2
ATOM	1747	O	SER	257	3.286	22.988	68.352	1.000	31.47			
ANISOU	1747	O	SER	257	2740	5886	3330	-435	-689	-	6	3
ATOM	1748	N	ARG	258	2.022	22.123	66.763	1.000	26.04			
ANISOU	1748	N	ARG	258	3257	4477	2161	-238	-441	-	1	9
ATOM	1749	CA	ARG	258	2.982	22.541	65.747	1.000	25.81			
ANISOU	1749	CA	ARG	258	2606	4735	2466	73	-338	-	1	9
ATOM	1750	C	ARG	258	2.321	22.609	64.383	1.000	18.26			
ANISOU	1750	C	ARG	258	2374	2541	2021	39	83	-	8	5
ATOM	1751	O	ARG	258	1.288	21.967	64.131	1.000	19.23			
ANISOU	1751	O	ARG	258	2600	2819	1888	-389	311	-	4	2
ATOM	1752	CB	ARG	258	4.188	21.592	65.664	1.000	29.78			
ANISOU	1752	CB	ARG	258	3403	5052	2861	695	-552	-	5	7
ATOM	1753	CG	ARG	258	4.246	20.784	64.384	1.000	32.64			
ANISOU	1753	CG	ARG	258	4358	4148	3896	146	97	-	5	6
ATOM	1754	CD	ARG	258	5.325	19.746	64.499	1.000	30.38			
ANISOU	1754	CD	ARG	258	3812	4423	3309	-57	341	-	1	6
ATOM	1755	NE	ARG	258	6.433	19.909	63.581	1.000	29.43			
ANISOU	1755	NE	ARG	258	3990	4604	2588	-22	70	5	4	2
ATOM	1756	CZ	ARG	258	6.453	19.389	62.359	1.000	25.02			
ANISOU	1756	CZ	ARG	258	2540	3893	3074	304	-243	1	0	4
ATOM	1757	NH1	ARG	258	5.456	18.677	61.835	1.000	22.88			
ANISOU	1757	NH1	ARG	258	2105	2607	3982	359	315	2	8	9
ATOM	1758	NH2	ARG	258	7.523	19.593	61.617	1.000	22.03			
ANISOU	1758	NH2	ARG	258	2477	2775	3120	-430	-287	-	9	6
ATOM	1759	N	THR	259	2.927	23.415	63.527	1.000	20.17			
ANISOU	1759	N	THR	259	2010	3640	2013	-743	91	-	1	0
ATOM	1760	CA	THR	259	2.485	23.505	62.138	1.000	18.33			
ANISOU	1760	CA	THR	259	1801	3043	2121	-533	43	-	6	8
ATOM	1761	CB	THR	259	1.821	24.821	61.713	1.000	23.23			
ANISOU	1761	CB	THR	259	2082	3169	3576	-384	-164	-	5	8
ATOM	1762	OG1	THR	259	2.839	25.830	61.681	1.000	34.27			
ANISOU	1762	OG1	THR	259	2181	2562	8277	-137	-996	-	7	9
ATOM	1763	CG2	THR	259	0.738	25.198	62.704	1.000	25.49			
ANISOU	1763	CG2	THR	259	4466	2233	2987	325	396	-	9	4
ATOM	1764	C	THR	259	3.702	23.352	61.222	1.000	18.44			
ANISOU	1764	C	THR	259	2035	2822	2150	-753	274	-	5	8
ATOM	1765	O	THR	259	4.835	23.698	61.603	1.000	24.74			
ANISOU	1765	O	THR	259	1961	5370	2069	-964	231	-	7	1
ATOM	1766	N	SER	260	3.420	22.867	60.026	1.000	16.29			
ANISOU	1766	N	SER	260	1971	2352	1864	-224	2	-	7	5
ATOM	1767	CA	SER	260	4.447	22.832	58.989	1.000	17.43			
ANISOU	1767	CA	SER	260	1783	2961	1879	321	-95	-	7	2
ATOM	1768	CB	SER	260	5.224	21.514	58.956	1.000	20.17			
ANISOU	1768	CB	SER	260	2306	3257	2100	762	-127	3	8	8
ATOM	1769	OG	SER	260	4.416	20.392	58.698	1.000	27.09			
ANISOU	1769	OG	SER	260	3651	2803	3839	426	217	5	5	4

- 148 -

ATOM	1770	C	SER	260	3.832	23.062	57.614	1.000	14.52
ANISOU	1770	C	SER	260	1463	2165	1889	83	-100 - 1
ATOM	1771	O	SER	260	2.686	22.681	57.402	1.000	15.92
ANISOU	1771	O	SER	260	1513	2489	2049	-93	-1 2 5 7
ATOM	1772	N	SER	261	4.617	23.660	56.742	1.000	13.45
ANISOU	1772	N	SER	261	1489	1832	1788	-190	-120 - 5 0 0
ATOM	1773	CA	SER	261	4.294	23.864	55.334	1.000	13.52
ANISOU	1773	CA	SER	261	1599	1726	1812	-204	30 - 3 1 5
ATOM	1774	C	SER	261	5.209	22.943	54.545	1.000	12.45
ANISOU	1774	C	SER	261	1332	1887	1513	-42	-240 - 1 6 1
ATOM	1775	O	SER	261	6.438	23.072	54.662	1.000	15.07
ANISOU	1775	O	SER	261	1344	1885	2497	-68	-331 - 3 4 3
ATOM	1776	CB	SER	261	4.446	25.330	54.943	1.000	17.76
ANISOU	1776	CB	SER	261	2718	1625	2404	-399	-485 - 3 1 8
ATOM	1777	OG	SER	261	4.428	25.554	53.570	1.000	27.54
ANISOU	1777	OG	SER	261	4342	3308	2814	-719	-821 9 5 5
ATOM	1778	N	VAL	262	4.623	22.045	53.782	1.000	10.90
ANISOU	1778	N	VAL	262	1215	1630	1299	41	-135 1 9
ATOM	1779	CA	VAL	262	5.393	21.031	53.026	1.000	11.61
ANISOU	1779	CA	VAL	262	1334	1634	1442	156	-103 1 7
ATOM	1780	CB	VAL	262	5.026	19.639	53.558	1.000	11.87
ANISOU	1780	CB	VAL	262	1262	1636	1614	9	-187 - 7 4
ATOM	1781	CG1	VAL	262	5.778	18.577	52.779	1.000	13.12
ANISOU	1781	CG1	VAL	262	1462	1527	1997	-2	185 5 1
ATOM	1782	CG2	VAL	262	5.262	19.564	55.062	1.000	17.08
ANISOU	1782	CG2	VAL	262	3390	1494	1604	-374	-245 3 9
ATOM	1783	C	VAL	262	5.096	21.149	51.543	1.000	11.18
ANISOU	1783	C	VAL	262	1026	1790	1431	1	-111 - 1 3 8
ATOM	1784	O	VAL	262	3.939	20.969	51.127	1.000	12.76
ANISOU	1784	O	VAL	262	1064	2137	1648	-251	-84 - 2 7 1
ATOM	1785	N	PHE	263	6.090	21.438	50.714	1.000	9.50
ANISOU	1785	N	PHE	263	995 1297	1316	-6	-210	-181
ATOM	1786	CA	PHE	263	5.933	21.637	49.288	1.000	9.61
ANISOU	1786	CA	PHE	263	1310	1017	1324	-6	-284 - 4 2
ATOM	1787	CB	PHE	263	6.486	23.002	48.848	1.000	10.94
ANISOU	1787	CB	PHE	263	1282	1055	1821	-50	-253 4
ATOM	1788	CG	PHE	263	6.150	23.399	47.418	1.000	10.35
ANISOU	1788	CG	PHE	263	779 1231	1921	-58	32	3 4 0
ATOM	1789	CD1	PHE	263	6.858	22.915	46.326	1.000	9.98
ANISOU	1789	CD1	PHE	263	766 1183	1841	-26	-101	2 4 0
ATOM	1790	CD2	PHE	263	5.106	24.277	47.148	1.000	11.95
ANISOU	1790	CD2	PHE	263	1229	1261	2052	245	-29 2 6 1
ATOM	1791	CE1	PHE	263	6.530	23.229	45.019	1.000	12.49
ANISOU	1791	CE1	PHE	263	1718	1173	1857	31	-370 1 3 6
ATOM	1792	CE2	PHE	263	4.769	24.601	45.836	1.000	13.12
ANISOU	1792	CE2	PHE	263	1451	1382	2151	43	-292 3 5 3
ATOM	1793	CZ	PHE	263	5.491	24.112	44.762	1.000	12.42
ANISOU	1793	CZ	PHE	263	1318	1453	1948	-138	-187 6 4 9
ATOM	1794	C	PHE	263	6.636	20.505	48.530	1.000	8.91
ANISOU	1794	C	PHE	263	1076	1085	1223	-39	-142 2 4
ATOM	1795	O	PHE	263	7.868	20.406	48.538	1.000	10.98
ANISOU	1795	O	PHE	263	1098	1233	1842	-120	-224 - 1 4 5
ATOM	1796	N	PHE	264	5.856	19.691	47.812	1.000	9.19
ANISOU	1796	N	PHE	264	1089	1266	1136	-86	-105 - 8 2
ATOM	1797	CA	PHE	264	6.386	18.602	46.991	1.000	9.64
ANISOU	1797	CA	PHE	264	1009	1238	1417	-56	-60 - 1 2 6
ATOM	1798	CB	PHE	264	5.483	17.358	47.005	1.000	9.92
ANISOU	1798	CB	PHE	264	1209	1201	1359	-78	17 9
ATOM	1799	CG	PHE	264	5.265	16.673	48.336	1.000	11.22
ANISOU	1799	CG	PHE	264	1241	1647	1374	-121	38 7 7
ATOM	1800	CD1	PHE	264	6.292	16.236	49.139	1.000	15.38

- 149 -

ANISOU 1800 CD1 PHE 264 1467 2641 1734 -225 -8 8 7 3
 ATOM 1801 CD2 PHE 264 3.988 16.433 48.808 1.000 16.96
 ANISOU 1801 CD2 PHE 264 1425 3252 1769 -610 -79 9 5 8
 ATOM 1802 CE1 PHE 264 6.090 15.596 50.336 1.000 14.52
 ANISOU 1802 CE1 PHE 264 1745 2417 1354 162 334 4 5 2
 ATOM 1803 CE2 PHE 264 3.755 15.796 50.019 1.000 18.04
 ANISOU 1803 CE2 PHE 264 1747 3405 1704 -590 -109 10 0 8
 ATOM 1804 CZ PHE 264 4.817 15.354 50.779 1.000 12.52
 ANISOU 1804 CZ PHE 264 1772 1536 1449 -57 227 3 3 4
 ATOM 1805 C PHE 264 6.535 19.038 45.533 1.000 8.98
 ANISOU 1805 C PHE 264 1103 919 1392 143 81 -9 2
 ATOM 1806 O PHE 264 5.497 19.368 44.930 1.000 9.79
 ANISOU 1806 O PHE 264 991 1190 1540 28 105 10 3
 ATOM 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43
 ANISOU 1807 N LEU 265 992 884 1325 173 -180 1 5 8
 ATOM 1808 CA LEU 265 7.984 19.224 43.566 1.000 8.66
 ANISOU 1808 CA LEU 265 883 1066 1339 63 -33 -7 6
 ATOM 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10
 ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 2 4 8
 ATOM 1810 CG LEU 265 9.570 20.351 41.871 1.000 9.37
 ANISOU 1810 CG LEU 265 1072 1009 1478 242 25 1 2 9
 ATOM 1811 CD1 LEU 265 8.725 21.522 41.408 1.000 10.80
 ANISOU 1811 CD1 LEU 265 1291 1004 1811 181 -114 2 9 6
 ATOM 1812 CD2 LEU 265 11.048 20.684 41.678 1.000 10.87
 ANISOU 1812 CD2 LEU 265 1129 1483 1519 134 43 1 4 6
 ATOM 1813 C LEU 265 7.933 17.849 42.875 1.000 10.21
 ANISOU 1813 C LEU 265 932 1188 1760 -6 -38 -3 0 2
 ATOM 1814 O LEU 265 8.858 17.043 43.042 1.000 10.45
 ANISOU 1814 O LEU 265 1388 969 1612 84 -217 1 0 7
 ATOM 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00
 ANISOU 1815 N ARG 266 1325 1069 1404 -120 -222 1 5
 ATOM 1816 CA ARG 266 6.572 16.198 41.628 1.000 10.50
 ANISOU 1816 CA ARG 266 1219 1217 1554 -294 110 -2 1 0
 ATOM 1817 CB ARG 266 5.208 15.675 42.124 1.000 10.56
 ANISOU 1817 CB ARG 266 978 1460 1574 -168 -103 -1 0 5
 ATOM 1818 CG ARG 266 4.965 15.894 43.609 1.000 11.24
 ANISOU 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6
 ATOM 1819 CD ARG 266 3.668 15.318 44.146 1.000 11.17
 ANISOU 1819 CD ARG 266 1113 1567 1564 -17 -49 -1 1
 ATOM 1820 NE ARG 266 2.508 15.879 43.447 1.000 9.43
 ANISOU 1820 NE ARG 266 1341 1157 1086 24 -100 -1 4 5
 ATOM 1821 CZ ARG 266 1.236 15.509 43.657 1.000 9.83
 ANISOU 1821 CZ ARG 266 1245 1194 1294 132 -159 -1
 ATOM 1822 NH1 ARG 266 0.961 14.567 44.572 1.000 11.20
 ANISOU 1822 NH1 ARG 266 1208 1240 1806 -144 -454 2 7 2
 ATOM 1823 NH2 ARG 266 0.225 16.048 42.975 1.000 11.08
 ANISOU 1823 NH2 ARG 266 1460 1265 1484 191 -283 7 3
 ATOM 1824 C ARG 266 6.601 16.190 40.099 1.000 10.28
 ANISOU 1824 C ARG 266 1273 1089 1545 -200 -5 -1 6 7
 ATOM 1825 O ARG 266 6.027 17.109 39.519 1.000 11.05
 ANISOU 1825 O ARG 266 1254 1153 1793 -132 47 -6 4
 ATOM 1826 N PRO 267 7.215 15.162 39.496 1.000 10.27
 ANISOU 1826 N PRO 267 1194 1239 1468 -33 130 3 2
 ATOM 1827 CD PRO 267 7.828 13.963 40.109 1.000 12.36
 ANISOU 1827 CD PRO 267 1865 1132 1697 -26 -529 -1 9 2
 ATOM 1828 CA PRO 267 7.304 15.157 38.036 1.000 10.12
 ANISOU 1828 CA PRO 267 1278 1095 1472 -129 38 -1 8 5
 ATOM 1829 CB PRO 267 8.250 13.986 37.767 1.000 11.83
 ANISOU 1829 CB PRO 267 1489 1088 1919 -72 90 -3 2 2
 ATOM 1830 CG PRO 267 8.017 13.053 38.913 1.000 10.72
 ANISOU 1830 CG PRO 267 960 1356 1755 95 -257 -1 8 7

- 150 -

ATOM	1831	C	PRO	267	5.977	14.929	37.344	1.000	10.86
ANISOU	1831	C	PRO	267	1330	1226	1570	-252	47 -161
ATOM	1832	O	PRO	267	5.030	14.421	37.934	1.000	12.03
ANISOU	1832	O	PRO	267	1316	1174	2080	-258	17 7 7
ATOM	1833	N	ASN	268	5.931	15.288	36.065	1.000	10.61
ANISOU	1833	N	ASN	268	1216	1146	1670	-70	-86 -129
ATOM	1834	CA	ASN	268	4.810	14.949	35.198	1.000	11.20
ANISOU	1834	CA	ASN	268	1285	1349	1622	-167	-43 -229
ATOM	1835	CB	ASN	268	4.954	15.664	33.846	1.000	14.02
ANISOU	1835	CB	ASN	268	2160	1410	1756	132	-316 2 3
ATOM	1836	CG	ASN	268	4.992	17.175	33.992	1.000	13.03
ANISOU	1836	CG	ASN	268	1811	1393	1747	189	-355 -88
ATOM	1837	OD1	ASN	268	4.046	17.748	34.566	1.000	16.65
ANISOU	1837	OD1	ASN	268	1910	1744	2673	292	-1 -159
ATOM	1838	ND2	ASN	268	6.037	17.818	33.495	1.000	14.19
ANISOU	1838	ND2	ASN	268	2505	1372	1516	161	264 -172
ATOM	1839	C	ASN	268	4.705	13.446	34.968	1.000	10.88
ANISOU	1839	C	ASN	268	1294	1314	1526	-75	-226 -164
ATOM	1840	O	ASN	268	5.715	12.732	34.979	1.000	11.68
ANISOU	1840	O	ASN	268	1534	1439	1464	87 -458	-121
ATOM	1841	N	ALA	269	3.484	12.980	34.688	1.000	12.22
ANISOU	1841	N	ALA	269	1484	1428	1732	-108	-397 -427
ATOM	1842	CA	ALA	269	3.277	11.547	34.417	1.000	12.12
ANISOU	1842	CA	ALA	269	1432	1356	1819	-238	-29 -282
ATOM	1843	CB	ALA	269	1.817	11.310	34.058	1.000	12.38
ANISOU	1843	CB	ALA	269	1439	1278	1985	-228	-183 2 9
ATOM	1844	C	ALA	269	4.125	10.981	33.283	1.000	11.26
ANISOU	1844	C	ALA	269	1445	1240	1592	25 -280	-141
ATOM	1845	O	ALA	269	4.493	9.800	33.263	1.000	12.53
ANISOU	1845	O	ALA	269	1428	1249	2085	-110	108 -188
ATOM	1846	N	ASP	270	4.438	11.799	32.276	1.000	11.47
ANISOU	1846	N	ASP	270	1701	1280	1378	-261	-341 -300
ATOM	1847	CA	ASP	270	5.214	11.378	31.113	1.000	11.92
ANISOU	1847	CA	ASP	270	1826	1106	1595	19 -183	-156
ATOM	1848	CB	ASP	270	4.760	12.096	29.850	1.000	14.13
ANISOU	1848	CB	ASP	270	1733	2038	1597	84 111 2 12	
ATOM	1849	CG	ASP	270	5.050	13.568	29.777	1.000	15.98
ANISOU	1849	CG	ASP	270	2309	1939	1823	418	-418 5 6 4
ATOM	1850	OD1	ASP	270	5.432	14.186	30.762	1.000	21.61
ANISOU	1850	OD1	ASP	270	4101	1797	2312	176	-515 1 6 3
ATOM	1851	OD2	ASP	270	4.880	14.152	28.674	1.000	24.64
ANISOU	1851	OD2	ASP	270	3995	3221	2145	-62	-169 13 9 5
ATOM	1852	C	ASP	270	6.721	11.542	31.264	1.000	12.86
ANISOU	1852	C	ASP	270	1840	1392	1654	-398	-61 3 1 5
ATOM	1853	O	ASP	270	7.443	11.290	30.292	1.000	14.83
ANISOU	1853	O	ASP	270	1813	2114	1709	-346	-141 4 9
ATOM	1854	N	PHE	271	7.230	11.911	32.439	1.000	11.85
ANISOU	1854	N	PHE	271	1360	1316	1824	59 -25 7 0	
ATOM	1855	CA	PHE	271	8.665	11.927	32.715	1.000	11.14
ANISOU	1855	CA	PHE	271	1242	1349	1641	10 230 1 6 2	
ATOM	1856	CB	PHE	271	8.972	12.378	34.143	1.000	12.19
ANISOU	1856	CB	PHE	271	1467	1444	1722	-96	-3 1 8 2
ATOM	1857	CG	PHE	271	10.385	11.992	34.597	1.000	12.77
ANISOU	1857	CG	PHE	271	1411	1640	1800	42 31 5 6	
ATOM	1858	CD1	PHE	271	11.475	12.488	33.904	1.000	13.22
ANISOU	1858	CD1	PHE	271	1513	1516	1993	168	220 4 9
ATOM	1859	CD2	PHE	271	10.624	11.155	35.666	1.000	13.55
ANISOU	1859	CD2	PHE	271	1343	1674	2131	139	84 2 5 5
ATOM	1860	CE1	PHE	271	12.779	12.178	34.249	1.000	14.26
ANISOU	1860	CE1	PHE	271	1432	1760	2225	-39	46 -4 1 6
ATOM	1861	CE2	PHE	271	11.925	10.806	36.019	1.000	15.88

- 151 -

ANISOU 1861 CE2 PHE 271 1537 1818 2679 -263 -675 2 6 0
 ATOM 1862 CZ PHE 271 13.006 11.288 35.304 1.000 14.15
 ANISOU 1862 CZ PHE 271 1166 1736 2475 7 -531 -467
 ATOM 1863 C PHE 271 9.259 10.550 32.410 1.000 11.27
 ANISOU 1863 C PHE 271 1359 1338 1585 75 271 3 4 8
 ATOM 1864 O PHE 271 8.785 9.531 32.920 1.000 12.97
 ANISOU 1864 O PHE 271 2011 1320 1596 -85 473 2 7 9
 ATOM 1865 N THR 272 10.261 10.498 31.541 1.000 11.95
 ANISOU 1865 N THR 272 1018 1503 2020 -214 300 -1 1 5
 ATOM 1866 CA THR 272 10.823 9.254 30.992 1.000 12.70
 ANISOU 1866 CA THR 272 1615 1557 1652 132 341 1 4 6
 ATOM 1867 CB THR 272 10.679 9.281 29.450 1.000 16.79
 ANISOU 1867 CB THR 272 1814 2829 1737 -595 157 -4 0 6
 ATOM 1868 OG1 THR 272 9.301 9.471 29.090 1.000 18.02
 ANISOU 1868 OG1 THR 272 1912 2921 2013 -497 -73 9 1
 ATOM 1869 CG2 THR 272 11.200 7.976 28.856 1.000 17.02
 ANISOU 1869 CG2 THR 272 2144 2857 1467 -475 538 -1 9 4
 ATOM 1870 C THR 272 12.272 9.057 31.423 1.000 12.02
 ANISOU 1870 C THR 272 1436 1573 1559 92 603 1 3 7
 ATOM 1871 O THR 272 13.055 10.031 31.437 1.000 14.17
 ANISOU 1871 O THR 272 1451 1583 2351 125 602 4 1 2
 ATOM 1872 N PHE 273 12.625 7.837 31.828 1.000 12.34
 ANISOU 1872 N PHE 273 1402 1585 1703 17 378 1 5 8
 ATOM 1873 CA PHE 273 13.953 7.492 32.312 1.000 12.20
 ANISOU 1873 CA PHE 273 1362 1364 1909 -126 336 1 4 7
 ATOM 1874 CB PHE 273 13.951 7.514 33.861 1.000 12.37
 ANISOU 1874 CB PHE 273 1362 1447 1890 -102 211 -8
 ATOM 1875 CG PHE 273 12.988 6.528 34.491 1.000 11.65
 ANISOU 1875 CG PHE 273 1398 1631 1396 -367 42 -2 1 5
 ATOM 1876 CD1 PHE 273 11.684 6.889 34.773 1.000 14.11
 ANISOU 1876 CD1 PHE 273 1531 2214 1614 -336 293 -6 2
 ATOM 1877 CD2 PHE 273 13.409 5.245 34.803 1.000 13.20
 ANISOU 1877 CD2 PHE 273 2024 1639 1352 -358 339 -9
 ATOM 1878 CE1 PHE 273 10.793 5.993 35.323 1.000 13.25
 ANISOU 1878 CE1 PHE 273 1536 2081 1418 -98 447 4 2
 ATOM 1879 CE2 PHE 273 12.530 4.329 35.327 1.000 13.39
 ANISOU 1879 CE2 PHE 273 1529 1905 1654 -224 140 2 8 3
 ATOM 1880 CZ PHE 273 11.227 4.706 35.604 1.000 14.75
 ANISOU 1880 CZ PHE 273 1444 2260 1902 -90 -186 2 7 5
 ATOM 1881 C PHE 273 14.423 6.135 31.795 1.000 12.45
 ANISOU 1881 C PHE 273 1278 1526 1927 -120 317 -3 1
 ATOM 1882 O PHE 273 13.645 5.311 31.291 1.000 11.95
 ANISOU 1882 O PHE 273 1590 1580 1370 -137 226 -1 3
 ATOM 1883 N SER 274 15.717 5.854 31.952 1.000 12.07
 ANISOU 1883 N SER 274 1270 1640 1677 -29 558 3 5 3
 ATOM 1884 CA SER 274 16.335 4.586 31.604 1.000 14.39
 ANISOU 1884 CA SER 274 1583 1534 2349 43 707 3 8 4
 ATOM 1885 CB SER 274 17.845 4.771 31.438 1.000 14.49
 ANISOU 1885 CB SER 274 1578 1727 2202 213 695 3 2 9
 ATOM 1886 OG SER 274 18.564 3.558 31.424 1.000 14.97
 ANISOU 1886 OG SER 274 1763 1848 2078 349 348 -1 3
 ATOM 1887 C SER 274 16.100 3.505 32.666 1.000 13.12
 ANISOU 1887 C SER 274 1670 1481 1833 8 461 1 3 7
 ATOM 1888 O SER 274 16.438 3.700 33.834 1.000 13.50
 ANISOU 1888 O SER 274 1493 1518 2116 -65 119 1 5
 ATOM 1889 N VAL 275 15.533 2.359 32.271 1.000 11.90
 ANISOU 1889 N VAL 275 1476 1618 1427 -110 490 1 9 5
 ATOM 1890 CA VAL 275 15.283 1.254 33.180 1.000 11.41
 ANISOU 1890 CA VAL 275 1708 1424 1204 -8 286 7 6
 ATOM 1891 CB VAL 275 14.346 0.198 32.543 1.000 12.74
 ANISOU 1891 CB VAL 275 1732 1300 1809 62 164 -1 6

- 152 -

ATOM	1892	CG1	VAL	275	14.157	-1.020	33.437	1.000	16.10	
ANISOU	1892	CG1	VAL	275	2352	1803	1962	-614	-663	3 7 0
ATOM	1893	CG2	VAL	275	12.961	0.763	32.261	1.000	13.81	
ANISOU	1893	CG2	VAL	275	1535	1786	1924	16	363	1 2 6
ATOM	1894	C	VAL	275	16.577	0.622	33.692	1.000	12.62	
ANISOU	1894	C	VAL	275	1574	1628	1594	14	375	1 3 6
ATOM	1895	O	VAL	275	16.729	0.405	34.926	1.000	13.01	
ANISOU	1895	O	VAL	275	1667	1643	1634	9	118	1 8 0
ATOM	1896	N	PRO	276	17.569	0.286	32.889	1.000	14.64	
ANISOU	1896	N	PRO	276	1583	2066	1914	2	454	- 4 2
ATOM	1897	CD	PRO	276	17.583	0.285	31.415	1.000	15.84	
ANISOU	1897	CD	PRO	276	1565	2536	1916	89	755	3 5
ATOM	1898	CA	PRO	276	18.827	-0.250	33.453	1.000	16.76	
ANISOU	1898	CA	PRO	276	1667	2403	2296	261	393	- 1 6 3
ATOM	1899	CB	PRO	276	19.732	-0.503	32.236	1.000	18.27	
ANISOU	1899	CB	PRO	276	1804	2568	2571	411	574	- 1 4 2
ATOM	1900	CG	PRO	276	18.868	-0.385	31.029	1.000	18.96	
ANISOU	1900	CG	PRO	276	2147	2763	2293	725	694	- 3 7
ATOM	1901	C	PRO	276	19.500	0.710	34.420	1.000	16.32	
ANISOU	1901	C	PRO	276	1521	2342	2336	115	237	6 7
ATOM	1902	O	PRO	276	20.035	0.277	35.456	1.000	16.78	
ANISOU	1902	O	PRO	276	1411	2689	2275	93	376	2 5 3
ATOM	1903	N	LEU	277	19.475	2.019	34.155	1.000	16.58	
ANISOU	1903	N	LEU	277	1835	2412	2052	-15	483	1 4 8
ATOM	1904	CA	LEU	277	20.142	2.919	35.099	1.000	17.70	
ANISOU	1904	CA	LEU	277	1990	2226	2511	-21	362	1 1 8
ATOM	1905	CB	LEU	277	20.298	4.277	34.425	1.000	20.20	
ANISOU	1905	CB	LEU	277	2952	2292	2432	-1	-14	2 7 1
ATOM	1906	CG	LEU	277	21.048	5.359	35.186	1.000	20.86	
ANISOU	1906	CG	LEU	277	2213	2221	3490	-32	-355	4 8 2
ATOM	1907	CD1	LEU	277	22.446	4.888	35.531	1.000	34.24	
ANISOU	1907	CD1	LEU	277	2157	2303	8552	69	-842	2 5 8
ATOM	1908	CD2	LEU	277	21.062	6.620	34.334	1.000	31.91	
ANISOU	1908	CD2	LEU	277	4745	2460	4918	-474	-572	1 1 5 0
ATOM	1909	C	LEU	277	19.411	2.989	36.430	1.000	16.55	
ANISOU	1909	C	LEU	277	1975	1885	2430	-218	211	- 2 4 3
ATOM	1910	O	LEU	277	19.997	3.116	37.517	1.000	19.19	
ANISOU	1910	O	LEU	277	2179	2636	2476	-617	50	1 2 2
ATOM	1911	N	ALA	278	18.080	2.905	36.386	1.000	15.48	
ANISOU	1911	N	ALA	278	2008	1904	1969	-358	279	1 1 2
ATOM	1912	CA	ALA	278	17.308	2.896	37.636	1.000	14.51	
ANISOU	1912	CA	ALA	278	2109	1763	1641	-309	74	1 6 7
ATOM	1913	CB	ALA	278	15.814	2.896	37.347	1.000	15.41	
ANISOU	1913	CB	ALA	278	2017	1773	2064	66	301	6 2 6
ATOM	1914	C	ALA	278	17.710	1.684	38.479	1.000	14.55	
ANISOU	1914	C	ALA	278	1972	1869	1689	-195	-255	7 9
ATOM	1915	O	ALA	278	17.894	1.770	39.683	1.000	13.80	
ANISOU	1915	O	ALA	278	1444	2144	1655	-250	-166	8 9
ATOM	1916	N	ARG	279	17.841	0.530	37.842	1.000	13.86	
ANISOU	1916	N	ARG	279	1795	1728	1742	-432	-128	1 6 9
ATOM	1917	CA	ARG	279	18.242	-0.679	38.560	1.000	15.88	
ANISOU	1917	CA	ARG	279	1995	1973	2064	59	355	4 1 1
ATOM	1918	CB	ARG	279	18.204	-1.922	37.648	1.000	16.83	
ANISOU	1918	CB	ARG	279	1889	1897	2609	84	544	2 5 0
ATOM	1919	CG	ARG	279	16.790	-2.323	37.291	1.000	19.63	
ANISOU	1919	CG	ARG	279	2123	2196	3139	-63	233	9 1
ATOM	1920	CD	ARG	279	16.656	-3.288	36.131	1.000	27.03	
ANISOU	1920	CD	ARG	279	3924	3198	3150	-603	-275	- 1 9 8
ATOM	1921	NE	ARG	279	17.236	-4.578	36.364	1.000	27.45	
ANISOU	1921	NE	ARG	279	4659	2854	2915	-359	751	- 7 8 9
ATOM	1922	CZ	ARG	279	16.714	-5.717	36.779	1.000	32.85	

- 153 -

ANISOU 1922 CZ ARG 279 4486 3045 4948 -475 448 -2 2 2
 ATOM 1923 NH1 ARG 279 15.424 -5.874 37.089 1.000 29.96
 ANISOU 1923 NH1 ARG 279 4653 2168 4562 -103 967 -6 7 8
 ATOM 1924 NH2 ARG 279 17.551 -6.750 36.890 1.000 37.87
 ANISOU 1924 NH2 ARG 279 4879 2436 7074 -276 3278 -8 2 4
 ATOM 1925 C ARG 279 19.628 -0.519 39.150 1.000 17.48
 ANISOU 1925 C ARG 279 2118 1653 2871 75 -8 7 0 5
 ATOM 1926 O ARG 279 19.916 -1.064 40.212 1.000 26.82
 ANISOU 1926 O ARG 279 3764 3102 3325 -1987 -1467 1 3 8 3
 ATOM 1927 N GLU 280 20.538 0.189 38.505 1.000 17.73
 ANISOU 1927 N GLU 280 1983 2293 2459 109 609 3 7
 ATOM 1928 CA GLU 280 21.899 0.317 39.026 1.000 19.66
 ANISOU 1928 CA GLU 280 2049 2023 3396 125 215 7 3 7
 ATOM 1929 CB GLU 280 22.836 0.886 37.936 1.000 20.17
 ANISOU 1929 CB GLU 280 1648 2457 3560 464 138 1 0 9 9
 ATOM 1930 CG GLU 280 22.964 -0.149 36.818 1.000 31.79
 ANISOU 1930 CG GLU 280 3477 4175 4427 801 1187 -4
 ATOM 1931 CD GLU 280 23.698 0.341 35.590 1.000 39.66
 ANISOU 1931 CD GLU 280 5144 5703 4221 -64 1339 -6
 ATOM 1932 OE1 GLU 280 24.466 1.327 35.685 1.000 39.65
 ANISOU 1932 OE1 GLU 280 3464 5891 5710 334 574 1 6 3 9
 ATOM 1933 OE2 GLU 280 23.489 -0.294 34.519 1.000 41.55
 ANISOU 1933 OE2 GLU 280 5257 6747 3781 2245 -184 1 0 2
 ATOM 1934 C GLU 280 21.984 1.188 40.266 1.000 19.68
 ANISOU 1934 C GLU 280 1488 2350 3640 -566 162 4 9 0
 ATOM 1935 O GLU 280 23.031 1.142 40.958 1.000 25.69
 ANISOU 1935 O GLU 280 1871 3766 4123 231 -245 1 8 0
 ATOM 1936 N CYS 281 20.943 1.980 40.565 1.000 18.57
 ANISOU 1936 N CYS 281 1560 2609 2887 -406 -211 1 7 6
 ATOM 1937 CA CYS 281 21.098 2.762 41.806 1.000 23.83
 ANISOU 1937 CA CYS 281 3222 2647 3184 -1189 176 -1 2 2
 ATOM 1938 CB CYS 281 21.079 4.264 41.523 1.000 25.40
 ANISOU 1938 CB CYS 281 3278 2655 3718 -426 368 -4 6
 ATOM 1939 SG CYS 281 19.587 4.904 40.763 1.000 27.05
 ANISOU 1939 SG CYS 281 3069 2914 4295 -522 -37 -7 9 4
 ATOM 1940 C CYS 281 20.098 2.406 42.907 1.000 16.99
 ANISOU 1940 C CYS 281 1377 1604 3475 109 -6 -5 4 6
 ATOM 1941 O CYS 281 19.971 3.173 43.889 1.000 17.04
 ANISOU 1941 O CYS 281 2294 1277 2902 -204 -484 -1 2 9
 ATOM 1942 N GLY 282 19.447 1.245 42.794 1.000 15.23
 ANISOU 1942 N GLY 282 1617 1597 2572 3 -58 -4 3 6
 ATOM 1943 CA GLY 282 18.731 0.674 43.914 1.000 15.61
 ANISOU 1943 CA GLY 282 1565 1973 2394 6 -331 -2 6 6
 ATOM 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75
 ANISOU 1944 C GLY 282 1635 1562 2029 -270 -446 -7 8
 ATOM 1945 O GLY 282 16.585 0.012 44.639 1.000 14.99
 ANISOU 1945 O GLY 282 1751 1630 2313 207 -242 4 5 5
 ATOM 1946 N PHE 283 16.744 1.009 42.582 1.000 12.65
 ANISOU 1946 N PHE 283 1434 1803 1570 -200 18 -2 5 2
 ATOM 1947 CA PHE 283 15.292 0.886 42.374 1.000 11.80
 ANISOU 1947 CA PHE 283 1477 1032 1974 -15 -264 4 6
 ATOM 1948 CB PHE 283 14.839 1.890 41.295 1.000 14.13
 ANISOU 1948 CB PHE 283 2262 972 2136 109 -187 1 5 9
 ATOM 1949 CG PHE 283 14.906 3.351 41.757 1.000 12.63
 ANISOU 1949 CG PHE 283 1711 1033 2055 47 -86 9
 ATOM 1950 CD1 PHE 283 13.851 3.928 42.409 1.000 13.45
 ANISOU 1950 CD1 PHE 283 1697 1399 2013 -166 24 -2 2 9
 ATOM 1951 CD2 PHE 283 16.037 4.111 41.519 1.000 13.15
 ANISOU 1951 CD2 PHE 283 1567 1135 2295 142 -41 -9 9
 ATOM 1952 CE1 PHE 283 13.903 5.248 42.839 1.000 15.61
 ANISOU 1952 CE1 PHE 283 2111 1649 2171 -202 484 -6 1 7

- 154 -

ATOM	1953	CE2	PHE	283	16.112	5.432	41.963	1.000	12.60	
ANISOU	1953	CE2	PHE	283	1783	937	2068	32	-18	2 6 4
ATOM	1954	CZ	PHE	283	15.040	5.993	42.641	1.000	13.37	
ANISOU	1954	CZ	PHE	283	1863	865	2352	187	-149	1 3
ATOM	1955	C	PHE	283	14.915	-0.534	41.972	1.000	11.23	
ANISOU	1955	C	PHE	283	1527	974	1765	63	-172	6 5
ATOM	1956	O	PHE	283	15.471	-1.071	40.990	1.000	13.24	
ANISOU	1956	O	PHE	283	1249	1428	2355	175	-120	-3 6 1
ATOM	1957	N	ASP	284	13.998	-1.130	42.712	1.000	12.31	
ANISOU	1957	N	ASP	284	1607	1333	1736		-268	-312 8 7
ATOM	1958	CA	ASP	284	13.589	-2.528	42.527	1.000	12.48	
ANISOU	1958	CA	ASP	284	1725	1202	1814		-148	-543 3 5 0
ATOM	1959	CB	ASP	284	13.159	-3.156	43.876	1.000	12.67	
ANISOU	1959	CB	ASP	284	2014	1145	1656		-50	-406 1 3 5
ATOM	1960	CG	ASP	284	13.261	-4.667	43.909	1.000	13.40	
ANISOU	1960	CG	ASP	284	2077	1171	1843	110		-419 3 6 3
ATOM	1961	OD1	ASP	284	13.861	-5.246	42.974	1.000	14.98	
ANISOU	1961	OD1	ASP	284	1956	1094	2640		-87	11 6 0
ATOM	1962	OD2	ASP	284	12.762	-5.306	44.883	1.000	15.79	
ANISOU	1962	OD2	ASP	284	2494	1539	1966		-330	-446 4 3 8
ATOM	1963	C	ASP	284	12.478	-2.641	41.510	1.000	10.82	
ANISOU	1963	C	ASP	284	1238	1387	1487		-205	-99 1 2 3
ATOM	1964	O	ASP	284	11.373	-3.100	41.777	1.000	12.28	
ANISOU	1964	O	ASP	284	1331	1175	2159		-209	48 1 9 1
ATOM	1965	N	VAL	285	12.751	-2.154	40.308	1.000	11.32	
ANISOU	1965	N	VAL	285	1204	1671	1426		-93	-48 6 1
ATOM	1966	CA	VAL	285	11.748	-2.062	39.260	1.000	11.45	
ANISOU	1966	CA	VAL	285	1468	1384	1500		39	-219 -1 5
ATOM	1967	CB	VAL	285	12.153	-1.072	38.157	1.000	11.58	
ANISOU	1967	CB	VAL	285	1412	1523	1465		-388	-428 - 8
ATOM	1968	CG1	VAL	285	12.278	0.362	38.679	1.000	15.02	
ANISOU	1968	CG1	VAL	285	2209	1458	2040		-264	-442 - 3 2
ATOM	1969	CG2	VAL	285	13.467	-1.482	37.495	1.000	15.70	
ANISOU	1969	CG2	VAL	285	1909	1443	2615		-159	309 4 4 7
ATOM	1970	C	VAL	285	11.424	-3.431	38.642	1.000	10.83	
ANISOU	1970	C	VAL	285	1232	1281	1602		93	-221 1 0 8
ATOM	1971	O	VAL	285	12.267	-4.301	38.520	1.000	12.13	
ANISOU	1971	O	VAL	285	1214	1192	2202		-28	300 1 6 2
ATOM	1972	N	SER	286	10.168	-3.523	38.248	1.000	11.09	
ANISOU	1972	N	SER	286	1116	1608	1489		-76	96 7
ATOM	1973	CA	SER	286	9.558	-4.622	37.510	1.000	11.32	
ANISOU	1973	CA	SER	286	1104	1479	1718		-41	-274 2 5 2
ATOM	1974	CB	SER	286	8.483	-5.292	38.344	1.000	9.88	
ANISOU	1974	CB	SER	286	1328	1141	1285		72	-207 7 0
ATOM	1975	OG	SER	286	7.570	-4.361	38.905	1.000	11.34	
ANISOU	1975	OG	SER	286	1391	1188	1729		147	-153 7 5
ATOM	1976	C	SER	286	9.019	-4.106	36.175	1.000	10.34	
ANISOU	1976	C	SER	286	1127	1227	1575		28	-87 2 4 5
ATOM	1977	O	SER	286	7.829	-4.112	35.869	1.000	12.62	
ANISOU	1977	O	SER	286	1223	2219	1353		0	-178 2 2 8
ATOM	1978	N	LEU	287	9.926	-3.622	35.335	1.000	12.45	
ANISOU	1978	N	LEU	287	1414	1664	1653		-212	3 1 6 1
ATOM	1979	CA	LEU	287	9.654	-2.900	34.099	1.000	12.59	
ANISOU	1979	CA	LEU	287	1622	1558	1605		-366	94 1 8 4
ATOM	1980	CB	LEU	287	10.145	-1.452	34.210	1.000	12.91	
ANISOU	1980	CB	LEU	287	1716	1591	1597		-373	-95 2 7
ATOM	1981	CG	LEU	287	9.452	-0.590	35.264	1.000	12.96	
ANISOU	1981	CG	LEU	287	1182	1848	1895		-407	-51 -17 0
ATOM	1982	CD1	LEU	287	10.229	0.708	35.484	1.000	13.34	
ANISOU	1982	CD1	LEU	287	1644	1108	2318		-38	-124 2 2 3
ATOM	1983	CD2	LEU	287	8.006	-0.248	34.914	1.000	14.56	

- 155 -

ANISOU	1983	CD2	LEU	287	1716	1548	2267	36	-550	3	1	8
ATOM	1984	C	LEU	287	10.319	-3.610	32.928	1.000	12	.63		
ANISOU	1984	C	LEU	287	1837	1244	1719	-233	248	3	5	4
ATOM	1985	O	LEU	287	11.529	-3.805	32.916	1.000	16	.68		
ANISOU	1985	O	LEU	287	1779	1998	2560	-292	390	-	1	4
ATOM	1986	N	ASP	288	9.531	-4.045	31.950	1.000	13	.91		
ANISOU	1986	N	ASP	288	2080	1751	1455	4	223	2	2	7
ATOM	1987	CA	ASP	288	10.079	-4.688	30.759	1.000	15	.50		
ANISOU	1987	CA	ASP	288	2029	2269	1593	-122	605	1	5	3
ATOM	1988	CB	ASP	288	8.979	-5.478	30.043	1.000	17	.00		
ANISOU	1988	CB	ASP	288	2722	2125	1613	-250	362	-	2	
ATOM	1989	CG	ASP	288	9.480	-6.452	29.014	1.000	19	.30		
ANISOU	1989	CG	ASP	288	2467	2980	1885	173	243	-	3	7
ATOM	1990	OD1	ASP	288	10.447	-7.183	29.292	1.000	25	.95		
ANISOU	1990	OD1	ASP	288	2812	3190	3856	501	-239	-	7	8
ATOM	1991	OD2	ASP	288	8.911	-6.508	27.907	1.000	31	.76		
ANISOU	1991	OD2	ASP	288	5375	4430	2260	1266	-849	-	1	1
ATOM	1992	C	ASP	288	10.654	-3.652	29.811	1.000	17	.08		
ANISOU	1992	C	ASP	288	2259	2631	1602	-263	248	5	3	4
ATOM	1993	O	ASP	288	10.197	-2.502	29.708	1.000	23	.31		
ANISOU	1993	O	ASP	288	4276	2268	2313	-244	-13	2	9	7
ATOM	1994	N	GLY	289	11.702	-3.966	29.049	1.000	21	.26		
ANISOU	1994	N	GLY	289	2748	3699	1632	-610	752	5	1	1
ATOM	1995	CA	GLY	289	12.116	-2.880	28.152	1.000	21	.65		
ANISOU	1995	CA	GLY	289	2842	3988	1396	-1163	71	6	2	6
ATOM	1996	C	GLY	289	13.084	-1.859	28.736	1.000	22	.09		
ANISOU	1996	C	GLY	289	2888	3509	1996	-738	-23	2	4	3
ATOM	1997	O	GLY	289	13.414	-1.836	29.924	1.000	20	.34		
ANISOU	1997	O	GLY	289	3230	2606	1891	-918	124	1	4	7
ATOM	1998	N	GLU	290	13.562	-0.952	27.869	1.000	16	.48		
ANISOU	1998	N	GLU	290	2665	2099	1496	5	222	-	4	4
ATOM	1999	CA	GLU	290	14.716	-0.117	28.182	1.000	16	.94		
ANISOU	1999	CA	GLU	290	2470	2161	1806	81	411	-	4	8
ATOM	2000	CB	GLU	290	15.579	0.012	26.912	1.000	20	.26		
ANISOU	2000	CB	GLU	290	2670	2740	2287	414	863	-	2	3
ATOM	2001	CG	GLU	290	16.071	-1.333	26.386	1.000	24	.53		
ANISOU	2001	CG	GLU	290	3251	3153	2916	664	1218	-	6	1
ATOM	2002	CD	GLU	290	16.812	-2.170	27.411	1.000	27	.91		
ANISOU	2002	CD	GLU	290	3019	3161	4424	989	940	-	2	5
ATOM	2003	OE1	GLU	290	17.874	-1.747	27.917	1.000	35	.13		
ANISOU	2003	OE1	GLU	290	3913	4458	4975	963	-85	-	8	7
ATOM	2004	OE2	GLU	290	16.336	-3.280	27.734	1.000	43	.76		
ANISOU	2004	OE2	GLU	290	6893	3257	6478	-30	-748	5	9	8
ATOM	2005	C	GLU	290	14.406	1.271	28.716	1.000	14	.67		
ANISOU	2005	C	GLU	290	2512	1756	1308	95	142	1	0	
ATOM	2006	O	GLU	290	15.260	1.840	29.412	1.000	15	.25		
ANISOU	2006	O	GLU	290	2074	1969	1750	50	418	-	2	6
ATOM	2007	N	THR	291	13.232	1.814	28.437	1.000	15	.72		
ANISOU	2007	N	THR	291	2173	2393	1406	78	346	-	5	1
ATOM	2008	CA	THR	291	12.792	3.087	28.991	1.000	15	.16		
ANISOU	2008	CA	THR	291	2080	1845	1833	-88	631	-	1	5
ATOM	2009	CB	THR	291	12.766	4.226	27.956	1.000	18	.67		
ANISOU	2009	CB	THR	291	2724	2529	1842	-361	769	3	3	6
ATOM	2010	OG1	THR	291	11.756	4.009	26.976	1.000	22	.93		
ANISOU	2010	OG1	THR	291	3313	3135	2265	445	78	1	4	6
ATOM	2011	CG2	THR	291	14.096	4.306	27.213	1.000	21	.82		
ANISOU	2011	CG2	THR	291	3035	2126	3130	357	1450	9	0	2
ATOM	2012	C	THR	291	11.402	2.920	29.622	1.000	12	.86		
ANISOU	2012	C	THR	291	1863	1604	1421	47	305	2	1	9
ATOM	2013	O	THR	291	10.625	2.024	29.270	1.000	16	.13		
ANISOU	2013	O	THR	291	2344	1983	1804	-303	750	-	4	3

- 156 -

ATOM	2014	N	ALA	292	11.037	3.791	30.542	1.000	12.41
ANISOU	2014	N	ALA	292	1495	1363	1859	-2	256 7 7
ATOM	2015	CA	ALA	292	9.746	3.839	31.202	1.000	11.57
ANISOU	2015	CA	ALA	292	1362	1257	1779	-213	153 3 7
ATOM	2016	CB	ALA	292	9.718	2.954	32.439	1.000	12.62
ANISOU	2016	CB	ALA	292	1768	1245	1784	100	357 4
ATOM	2017	C	ALA	292	9.385	5.255	31.614	1.000	10.32
ANISOU	2017	C	ALA	292	1317	1335	1270	-181	99 5 4
ATOM	2018	O	ALA	292	10.266	6.134	31.701	1.000	10.97
ANISOU	2018	O	ALA	292	1389	1138	1641	-146	279 1 0 4
ATOM	2019	N	THR	293	8.091	5.445	31.882	1.000	12.32
ANISOU	2019	N	THR	293	1486	1547	1647	-314	563 - 2 8 4
ATOM	2020	CA	THR	293	7.626	6.715	32.421	1.000	12.28
ANISOU	2020	CA	THR	293	1717	1460	1489	-168	337 - 2 0 0
ATOM	2021	CB	THR	293	6.352	7.215	31.733	1.000	13.27
ANISOU	2021	CB	THR	293	2128	1182	1730	-258	-159 - 2 8 4
ATOM	2022	OG1	THR	293	5.317	6.237	31.911	1.000	13.85
ANISOU	2022	OG1	THR	293	1831	1217	2216	8	-131 7 4
ATOM	2023	CG2	THR	293	6.474	7.303	30.212	1.000	13.72
ANISOU	2023	CG2	THR	293	1791	1683	1738	-252	-56 - 4 0 5
ATOM	2024	C	THR	293	7.363	6.635	33.937	1.000	10.58
ANISOU	2024	C	THR	293	1439	1050	1533	12	447 9
ATOM	2025	O	THR	293	7.211	5.576	34.553	1.000	10.29
ANISOU	2025	O	THR	293	1049	1102	1758	-56	93 1 1 8
ATOM	2026	N	PHE	294	7.243	7.810	34.569	1.000	11.53
ANISOU	2026	N	PHE	294	1794	1093	1494	-307	306 - 6 6
ATOM	2027	CA	PHE	294	6.806	7.939	35.950	1.000	10.41
ANISOU	2027	CA	PHE	294	1432	1061	1463	-174	125 - 1 6 2
ATOM	2028	CB	PHE	294	6.709	9.426	36.336	1.000	12.25
ANISOU	2028	CB	PHE	294	1930	1030	1694	-164	292 - 6 4
ATOM	2029	CG	PHE	294	6.270	9.658	37.770	1.000	12.77
ANISOU	2029	CG	PHE	294	1880	1136	1837	-103	178 - 4 2 7
ATOM	2030	CD1	PHE	294	7.123	9.462	38.839	1.000	14.73
ANISOU	2030	CD1	PHE	294	1976	1893	1727	-539	161 - 1 3 2
ATOM	2031	CD2	PHE	294	4.989	10.068	38.056	1.000	16.59
ANISOU	2031	CD2	PHE	294	2180	1923	2199	348	386 - 4 9 2
ATOM	2032	CE1	PHE	294	6.726	9.673	40.144	1.000	14.36
ANISOU	2032	CE1	PHE	294	1598	2028	1830	-505	280 - 1 1 8
ATOM	2033	CE2	PHE	294	4.575	10.275	39.345	1.000	16.75
ANISOU	2033	CE2	PHE	294	2214	2062	2087	692	144 - 6 0 2
ATOM	2034	CZ	PHE	294	5.426	10.065	40.413	1.000	15.17
ANISOU	2034	CZ	PHE	294	2040	1426	2296	327	97 - 1 3 5
ATOM	2035	C	PHE	294	5.484	7.195	36.172	1.000	10.89
ANISOU	2035	C	PHE	294	1401	1200	1536	-155	78 1 3 7
ATOM	2036	O	PHE	294	5.325	6.425	37.125	1.000	10.67
ANISOU	2036	O	PHE	294	1396	1297	1360	90	337 1 0 5
ATOM	2037	N	GLN	295	4.487	7.355	35.299	1.000	10.62
ANISOU	2037	N	GLN	295	1399	1187	1450	-18	88 - 2 4
ATOM	2038	CA	GLN	295	3.217	6.612	35.393	1.000	11.31
ANISOU	2038	CA	GLN	295	1433	1205	1660	-96	120 - 3 2 1
ATOM	2039	CB	GLN	295	2.284	7.053	34.254	1.000	11.66
ANISOU	2039	CB	GLN	295	1425	1053	1953	-25	63 - 1 4 1
ATOM	2040	CG	GLN	295	0.951	6.360	34.200	1.000	11.05
ANISOU	2040	CG	GLN	295	1573	1011	1614	-93	-118 1 8
ATOM	2041	CD	GLN	295	0.052	6.843	33.087	1.000	11.35
ANISOU	2041	CD	GLN	295	1592	1326	1395	173	57 - 1 3
ATOM	2042	OE1	GLN	295	0.349	7.823	32.378	1.000	15.06
ANISOU	2042	OE1	GLN	295	2306	1589	1825	110	7 3 7 9
ATOM	2043	NE2	GLN	295	-1.053	6.153	32.914	1.000	13.90
ANISOU	2043	NE2	GLN	295	1511	1757	2015	156	-282 2 0 8
ATOM	2044	C	GLN	295	3.412	5.107	35.389	1.000	10.12

- 157 -

ANISOU	2044	C	GLN	295	1154	1203	1486	21	160	-1	91
ATOM	2045	O	GLN	295	2.827	4.309	36.128	1.000	11	.82	
ANISOU	2045	O	GLN	295	1264	1542	1686	-107	41	1	3 7
ATOM	2046	N	ASP	296	4.267	4.558	34.538	1.000	9	.3 5	
ANISOU	2046	N	ASP	296	1076	1056	1422	-118	-76	-2	7 5
ATOM	2047	CA	ASP	296	4.655	3.172	34.416	1.000	9	.91	
ANISOU	2047	CA	ASP	296	1241	1139	1387	56	60	-2	4 3
ATOM	2048	CB	ASP	296	5.699	2.852	33.347	1.000	10	.2 6	
ANISOU	2048	CB	ASP	296	1315	1156	1429	113	132	-3	6
ATOM	2049	CG	ASP	296	5.343	2.981	31.885	1.000	11	.4 2	
ANISOU	2049	CG	ASP	296	1357	1578	1405	358	121	-1	9 9
ATOM	2050	OD1	ASP	296	4.143	2.904	31.531	1.000	13	.8 2	
ANISOU	2050	OD1	ASP	296	1511	1744	1997	149	-209	-6	2
ATOM	2051	OD2	ASP	296	6.282	3.151	31.047	1.000	13	.4 8	
ANISOU	2051	OD2	ASP	296	1802	1758	1564	228	364	7	3
ATOM	2052	C	ASP	296	5.175	2.682	35.770	1.000	10	.3 1	
ANISOU	2052	C	ASP	296	1416	1141	1361	16	91	-1	9 8
ATOM	2053	O	ASP	296	4.852	1.551	36.197	1.000	11	.4 0	
ANISOU	2053	O	ASP	296	1428	1452	1453	-288	32	3	5
ATOM	2054	N	TRP	297	6.004	3.484	36.441	1.000	10	.8 8	
ANISOU	2054	N	TRP	297	1752	1144	1238	-161	11	5	5
ATOM	2055	CA	TRP	297	6.646	3.104	37.685	1.000	11	.2 6	
ANISOU	2055	CA	TRP	297	1768	1215	1294	-217	-57	4	5
ATOM	2056	CB	TRP	297	7.899	3.999	37.890	1.000	10	.3 1	
ANISOU	2056	CB	TRP	297	1387	1417	1112	-87	213	1	2 0
ATOM	2057	CG	TRP	297	8.621	3.651	39.172	1.000	10	.9 8	
ANISOU	2057	CG	TRP	297	1456	1394	1324	164	-29	-4	3
ATOM	2058	CD2	TRP	297	9.082	4.534	40.202	1.000	12	.4 9	
ANISOU	2058	CD2	TRP	297	1255	1729	1761	75	-298	-1	9 7
ATOM	2059	CE2	TRP	297	9.692	3.755	41.201	1.000	16	.0 8	
ANISOU	2059	CE2	TRP	297	1860	2049	2202	-294	-977	4	9
ATOM	2060	CE3	TRP	297	9.040	5.910	40.379	1.000	17	.4 1	
ANISOU	2060	CE3	TRP	297	2778	1740	2096	-388	-916	-2	3 4
ATOM	2061	CD1	TRP	297	8.969	2.400	39.589	1.000	13	.5 8	
ANISOU	2061	CD1	TRP	297	1617	1518	2025	0	-664	1	1 4
ATOM	2062	NE1	TRP	297	9.614	2.444	40.808	1.000	16	.1 2	
ANISOU	2062	NE1	TRP	297	2165	1909	2051	-22	-873	2	2 0
ATOM	2063	CZ2	TRP	297	10.243	4.320	42.341	1.000	19	.8 5	
ANISOU	2063	CZ2	TRP	297	2756	2383	2404	-951	-1337	2	6 7
ATOM	2064	CZ3	TRP	297	9.586	6.466	41.515	1.000	23	.4 0	
ANISOU	2064	CZ3	TRP	297	4215	2030	2645	-1001	-1757	-7	7
ATOM	2065	CH2	TRP	297	10.181	5.670	42.486	1.000	21	.5 1	
ANISOU	2065	CH2	TRP	297	3178	2457	2537	-910	-1473	-5	1
ATOM	2066	C	TRP	297	5.700	3.138	38.882	1.000	10	.3 9	
ANISOU	2066	C	TRP	297	1172	1448	1329	-280	-237	3	9 1
ATOM	2067	O	TRP	297	5.574	2.159	39.639	1.000	13	.5 2	
ANISOU	2067	O	TRP	297	1748	1830	1557	32	-91	7	0 3
ATOM	2068	N	ILE	298	5.033	4.272	39.079	1.000	12	.0 8	
ANISOU	2068	N	ILE	298	1400	1710	1480	-49	83	4	5 1
ATOM	2069	CA	ILE	298	4.223	4.521	40.272	1.000	13	.4 3	
ANISOU	2069	CA	ILE	298	1301	2484	1317	-199	-158	-3	3
ATOM	2070	CB	ILE	298	4.370	5.988	40.689	1.000	16	.9 7	
ANISOU	2070	CB	ILE	298	1877	2908	1661	-1000	214	-6	3 0
ATOM	2071	CG2	ILE	298	3.538	6.423	41.876	1.000	22	.0 1	
ANISOU	2071	CG2	ILE	298	3980	3121	1263	-233	546	-3	3 9
ATOM	2072	CG1	ILE	298	5.847	6.253	41.037	1.000	27	.1 0	
ANISOU	2072	CG1	ILE	298	2588	5151	2557	-2140	-708	9	7
ATOM	2073	CD1	ILE	298	6.365	5.522	42.266	1.000	43	.1 3	
ANISOU	2073	CD1	ILE	298	5185	8299	2904	-3717	-3055	7	0 8
ATOM	2074	C	ILE	298	2.772	4.116	40.131	1.000	10	.9 4	
ANISOU	2074	C	ILE	298	1350	1652	1156	-165	-79	9	6

- 158 -

ATOM 2075 O ILE 298 2.137 3.844 41.155 1.000 12.67
 ANISOU 2075 O ILE 298 1689 1634 1493 -102 212 3 5 2
 ATOM 2076 N GLY 299 2.267 4.077 38.897 1.000 10.14
 ANISOU 2076 N GLY 299 1412 1057 1384 -51 -377 2 0 1
 ATOM 2077 CA GLY 299 0.866 3.822 38.695 1.000 10.72
 ANISOU 2077 CA GLY 299 1335 1084 1655 0 -229 -2 0 6
 ATOM 2078 C GLY 299 0.049 5.054 38.369 1.000 12.05
 ANISOU 2078 C GLY 299 1422 1293 1864 105 -292 0
 ATOM 2079 O GLY 299 0.585 6.088 37.976 1.000 13.11
 ANISOU 2079 O GLY 299 1917 1199 1866 174 80 -2 3
 ATOM 2080 N GLY 300 -1.268 4.931 38.490 1.000 13.92
 ANISOU 2080 N GLY 300 1393 1531 2363 182 -410 -2 2 3
 ATOM 2081 CA GLY 300 -2.237 5.932 38.087 1.000 14.02
 ANISOU 2081 CA GLY 300 1524 1471 2331 217 -563 -3 3 6
 ATOM 2082 C GLY 300 -2.587 7.015 39.074 1.000 11.97
 ANISOU 2082 C GLY 300 940 1603 2004 67 -488 -2 9 5
 ATOM 2083 O GLY 300 -3.322 7.950 38.722 1.000 10.90
 ANISOU 2083 O GLY 300 1219 1408 1515 -37 -203 -1 3 4
 ATOM 2084 N ASN 301 -2.090 6.910 40.285 1.000 11.64
 ANISOU 2084 N ASN 301 948 1557 1917 -383 -327 1 6 5
 ATOM 2085 CA ASN 301 -2.195 7.915 41.323 1.000 13.39
 ANISOU 2085 CA ASN 301 1626 1904 1557 -191 -403 1 8 3
 ATOM 2086 CB ASN 301 -3.047 7.301 42.427 1.000 17.60
 ANISOU 2086 CB ASN 301 1391 2869 2426 -9 326 2 2 8
 ATOM 2087 CG ASN 301 -4.021 8.196 43.108 1.000 19.15
 ANISOU 2087 CG ASN 301 2549 2827 1900 805 59 3 7 7
 ATOM 2088 OD1 ASN 301 -5.072 8.606 42.591 1.000 15.47
 ANISOU 2088 OD1 ASN 301 1258 2340 2280 -253 339 -8
 ATOM 2089 ND2 ASN 301 -3.661 8.510 44.367 1.000 29.28
 ANISOU 2089 ND2 ASN 301 3585 4783 2758 1521 -850 -8 8 5
 ATOM 2090 C ASN 301 -0.862 8.331 41.914 1.000 11.31
 ANISOU 2090 C ASN 301 1436 1669 1194 1 1 -1 6 8
 ATOM 2091 O ASN 301 -0.033 7.456 42.221 1.000 12.03
 ANISOU 2091 O ASN 301 1483 1548 1542 -151 -279 8 2
 ATOM 2092 N TYR 302 -0.634 9.628 42.133 1.000 11.53
 ANISOU 2092 N TYR 302 1186 1584 1611 -61 26 1 0 2
 ATOM 2093 CA TYR 302 0.573 10.046 42.838 1.000 11.90
 ANISOU 2093 CA TYR 302 1260 1395 1865 5 -212 2 2 5
 ATOM 2094 CB TYR 302 0.657 11.589 43.036 1.000 13.14
 ANISOU 2094 CB TYR 302 1768 1404 1820 -273 190 1 8 1
 ATOM 2095 CG TYR 302 1.082 12.287 41.750 1.000 10.88
 ANISOU 2095 CG TYR 302 1395 1347 1393 -321 2 -1 5 3
 ATOM 2096 CD1 TYR 302 2.421 12.439 41.413 1.000 11.29
 ANISOU 2096 CD1 TYR 302 1385 1246 1659 -58 98 -4 6
 ATOM 2097 CE1 TYR 302 2.859 13.075 40.248 1.000 10.60
 ANISOU 2097 CE1 TYR 302 1055 1241 1732 -11 52 -1
 ATOM 2098 CD2 TYR 302 0.161 12.793 40.858 1.000 11.30
 ANISOU 2098 CD2 TYR 302 1304 1332 1656 -145 105 -2 6
 ATOM 2099 CE2 TYR 302 0.573 13.406 39.690 1.000 11.72
 ANISOU 2099 CE2 TYR 302 1013 1733 1708 -288 -138 1 6 1
 ATOM 2100 CZ TYR 302 1.907 13.551 39.375 1.000 10.35
 ANISOU 2100 CZ TYR 302 1009 1214 1709 -229 -50 -1 9
 ATOM 2101 OH TYR 302 2.284 14.153 38.202 1.000 11.82
 ANISOU 2101 OH TYR 302 1192 1532 1766 -8 102 1 0 4
 ATOM 2102 C TYR 302 0.654 9.349 44.196 1.000 12.45
 ANISOU 2102 C TYR 302 1517 1450 1765 -181 -202 2 1 7
 ATOM 2103 O TYR 302 -0.375 9.230 44.878 1.000 13.55
 ANISOU 2103 O TYR 302 1464 1925 1759 -339 -211 7
 ATOM 2104 N VAL 303 1.868 8.967 44.542 1.000 12.06
 ANISOU 2104 N VAL 303 1517 1653 1413 -135 -3 3 4 0
 ATOM 2105 CA VAL 303 2.309 8.430 45.820 1.000 11.88

- 159 -

ANISOU	2105	CA	VAL	303	1434	1609	1471	-368	-197	2	2	3
ATOM	2106	CB	VAL	303	2.755	6.967	45.736	1.000	14.57			
ANISOU	2106	CB	VAL	303	1395	1682	2459	-217	-918	3	1	2
ATOM	2107	CG1	VAL	303	3.131	6.462	47.132	1.000	17.33			
ANISOU	2107	CG1	VAL	303	2644	1608	2331	-48	-1114	6	1	
ATOM	2108	CG2	VAL	303	1.703	6.041	45.122	1.000	14.80			
ANISOU	2108	CG2	VAL	303	1876	1676	2069	-592	-639	3	2	2
ATOM	2109	C	VAL	303	3.467	9.328	46.303	1.000	13.88			
ANISOU	2109	C	VAL	303	870 1791		2613 75	-286	-375			
ATOM	2110	O	VAL	303	4.526	9.417	45.681	1.000	19.70			
ANISOU	2110	O	VAL	303	1064	2307	4114	-61	323	-9	9	9
ATOM	2111	N	ASN	304	3.271	10.046	47.393	1.000	13.77			
ANISOU	2111	N	ASN	304	1681	1815	1737	-479	-388	1	4	0
ATOM	2112	CA	ASN	304	4.205	11.077	47.828	1.000	13.37			
ANISOU	2112	CA	ASN	304	1626	1240	2212	-213	-533	2	7	9
ATOM	2113	CB	ASN	304	3.460	12.223	48.566	1.000	13.24			
ANISOU	2113	CB	ASN	304	1206	1454	2370	-243	-344	2	9	6
ATOM	2114	CG	ASN	304	2.457	12.922	47.667	1.000	14.16			
ANISOU	2114	CG	ASN	304	1142	2326	1910	146	-88	2	3	0
ATOM	2115	OD1	ASN	304	2.776	13.283	46.540	1.000	16.65			
ANISOU	2115	OD1	ASN	304	1408	2456	2464	107	185	9	1	6
ATOM	2116	ND2	ASN	304	1.263	13.126	48.209	1.000	17.45			
ANISOU	2116	ND2	ASN	304	1414	2961	2257	545	181	3	1	5
ATOM	2117	C	ASN	304	5.325	10.588	48.728	1.000	11.18			
ANISOU	2117	C	ASN	304	1382	1299	1566	-183	-163	1	1	2
ATOM	2118	O	ASN	304	6.396	11.232	48.699	1.000	12.07			
ANISOU	2118	O	ASN	304	1325	1382	1879	-167	-66	-5	9	
ATOM	2119	N	ILE	305	5.092	9.541	49.516	1.000	12.56			
ANISOU	2119	N	ILE	305	1791	1296	1685	-152	-232	2	0	2
ATOM	2120	CA	ILE	305	6.063	9.011	50.463	1.000	14.01			
ANISOU	2120	CA	ILE	305	2314	1393	1614	-55	-479	7	9	
ATOM	2121	CB	ILE	305	5.781	9.493	51.906	1.000	14.44			
ANISOU	2121	CB	ILE	305	2223	1604	1659	-29	-217	1	5	7
ATOM	2122	CG2	ILE	305	5.725	11.017	51.956	1.000	15.31			
ANISOU	2122	CG2	ILE	305	1768	1608	2441	43 -479	-31	4		
ATOM	2123	CG1	ILE	305	4.543	8.853	52.498	1.000	14.83			
ANISOU	2123	CG1	ILE	305	1779	1694	2163	27 -307	-15	3		
ATOM	2124	CD1	ILE	305	4.163	9.252	53.900	1.000	28.68			
ANISOU	2124	CD1	ILE	305	3788	5324	1786	-1491	381	9	2	
ATOM	2125	C	ILE	305	6.059	7.487	50.389	1.000	12.79			
ANISOU	2125	C	ILE	305	1703	1355	1800	-260	-586	2	3	1
ATOM	2126	O	ILE	305	5.111	6.864	49.897	1.000	15.63			
ANISOU	2126	O	ILE	305	1779	1564	2597	-185	-1008	2	7	7
ATOM	2127	N	ARG	306	7.170	6.896	50.829	1.000	13.04			
ANISOU	2127	N	ARG	306	1618	1389	1946	-368	-598	3	8	3
ATOM	2128	CA	ARG	306	7.340	5.435	50.868	1.000	11.82			
ANISOU	2128	CA	ARG	306	1352	1366	1773	-375	-154	4	4	4
ATOM	2129	CB	ARG	306	8.111	4.965	49.640	1.000	15.28			
ANISOU	2129	CB	ARG	306	1976	1941	1886	-368	-19	1	1	1
ATOM	2130	CG	ARG	306	8.203	3.472	49.395	1.000	17.16			
ANISOU	2130	CG	ARG	306	2566	1953	2001	-68	-68	7	6	
ATOM	2131	CD	ARG	306	8.344	3.075	47.937	1.000	19.51			
ANISOU	2131	CD	ARG	306	2921	2361	2130	-397	-396	-3	0	2
ATOM	2132	NE	ARG	306	7.078	3.198	47.212	1.000	20.65			
ANISOU	2132	NE	ARG	306	2693	2844	2309	-1056	-310	2	1	4
ATOM	2133	CZ	ARG	306	6.948	3.186	45.893	1.000	17.11			
ANISOU	2133	CZ	ARG	306	2006	2225	2268	45 -91	5	9	6	
ATOM	2134	NH1	ARG	306	8.013	3.065	45.083	1.000	21.58			
ANISOU	2134	NH1	ARG	306	2405	2677	3116	-232	381	-6	6	9
ATOM	2135	NH2	ARG	306	5.734	3.301	45.365	1.000	17.51			
ANISOU	2135	NH2	ARG	306	2235	1550	2868	150	-484	-1	6	2

- 160 -

ATOM	2136	C	ARG	306	8.035	5.027	52.155	1.000	13.45	
ANISOU	2136	C	ARG	306	2254	1018	1837	-246	-481	9 8
ATOM	2137	O	ARG	306	9.006	5.682	52.556	1.000	12.15	
ANISOU	2137	O	ARG	306	1902	1099	1615	-18	-362	- 8 0
ATOM	2138	N	ARG	307	7.571	3.968	52.811	1.000	18.19	
ANISOU	2138	N	ARG	307	3073	1620	2218	-734	-938	7 9 2
ATOM	2139	CA	ARG	307	8.197	3.380	53.989	1.000	19.20	
ANISOU	2139	CA	ARG	307	3053	1963	2277	-675	-1236	6 4 3
ATOM	2140	C	ARG	307	9.086	2.191	53.611	1.000	23.08	
ANISOU	2140	C	ARG	307	4018	1905	2847	-270	-1885	3 2 9
ATOM	2141	O	ARG	307	8.636	1.292	52.895	1.000	35.93	
ANISOU	2141	O	ARG	307	6003	2403	5244	38	-3227	- 7 9 1
ATOM	2142	CB	ARG	307	7.131	2.918	54.997	1.000	28.25	
ANISOU	2142	CB	ARG	307	5557	3297	1882	-1503	-277	5 0 9
ATOM	2143	CG	ARG	307	6.032	3.921	55.275	1.000	33.39	
ANISOU	2143	CG	ARG	307	4564	4859	3261	-1613	731	2 0 8
ATOM	2144	CD	ARG	307	5.022	3.523	56.317	1.000	40.42	
ANISOU	2144	CD	ARG	307	6335	5701	3322	-1900	1263	9 7 1
ATOM	2145	NE	ARG	307	5.605	2.952	57.529	1.000	50.83	
ANISOU	2145	NE	ARG	307	8119	7287	3908	-2786	105	1 6 2 4
ATOM	2146	CZ	ARG	307	4.894	2.441	58.530	1.000	51.36	
ANISOU	2146	CZ	ARG	307	7424	8064	4025	-3650	-966	2 4 5 1
ATOM	2147	NH1	ARG	307	3.567	2.422	58.485	1.000	69.51	
ANISOU	2147	NH1	ARG	307	7586	10951	7874	-6970	-2008	3 2 4 5
ATOM	2148	NH2	ARG	307	5.489	1.937	59.600	1.000	59.99	
ANISOU	2148	NH2	ARG	307	10714	8150	3930	-5986	-3291	2 0 2 8
ATOM	2149	N	THR	308	10.347	2.147	54.048	1.000	22.92	
ANISOU	2149	N	THR	308	2759	2587	3364	-589	-200	1 7 0
ATOM	2150	CA	THR	308	11.215	1.009	53.794	1.000	24.47	
ANISOU	2150	CA	THR	308	3382	2649	3268	-360	52	1 5 0
ATOM	2151	C	THR	308	10.602	-0.252	54.382	1.000	31.10	
ANISOU	2151	C	THR	308	5251	2520	4044	-768	16	2 7 9
ATOM	2152	O	THR	308	10.610	-1.292	53.718	1.000	31.44	
ANISOU	2152	O	THR	308	4573	2676	4696	-457	-1745	- 4 0
ATOM	2153	CB	THR	308	12.615	1.279	54.378	1.000	23.51	
ANISOU	2153	CB	THR	308	3718	2086	3131	413	-694	5 4 2
ATOM	2154	OG1	THR	308	13.195	2.410	53.705	1.000	23.61	
ANISOU	2154	OG1	THR	308	2711	2503	3754	153	437	- 9
ATOM	2155	CG2	THR	308	13.573	0.141	54.117	1.000	26.37	
ANISOU	2155	CG2	THR	308	4427	2796	2796	927	-329	- 1 8
ATOM	2156	N	SER	309	10.066	-0.156	55.596	1.000	28.39	
ANISOU	2156	N	SER	309	3759	2774	4252	-19	2	1 3 0 0
ATOM	2157	CA	SER	309	9.488	-1.335	56.238	1.000	34.69	
ANISOU	2157	CA	SER	309	6110	3146	3925	-1066	-1089	1 6 2 6
ATOM	2158	C	SER	309	8.109	-1.737	55.724	1.000	41.41	
ANISOU	2158	C	SER	309	6442	3910	5383	-2171	-1170	2 1 4 4
ATOM	2159	O	SER	309	7.672	-2.884	55.952	1.000	57.05	
ANISOU	2159	O	SER	309	11389	5141	5146	-4907	-2077	2 0 2 7
ATOM	2160	CB	SER	309	9.450	-1.104	57.755	1.000	31.61	
ANISOU	2160	CB	SER	309	4863	2958	4188	-483	368	9 6 2
ATOM	2161	OG	SER	309	8.485	-0.135	58.107	1.000	38.99	
ANISOU	2161	OG	SER	309	4731	3477	6604	313	-2249	- 4 9 6
ATOM	2162	N	LYS	310	7.391	-0.868	55.032	1.000	47.69	
ANISOU	2162	N	LYS	310	5502	5577	7040	-539	-1369	1 5 8 3
ATOM	2163	FE	IUM	312	8.574	13.466	54.055	1.000	11.05	
ANISOU	2163	FE	IUM	312	1690	1156	1351	-101	-237	7 1
ATOM	2164	C1	AKG	313	5.987	14.815	54.612	1.000	19.65	
ANISOU	2164	C1	AKG	313	2777	2119	2572	258	-117	5 5 6
ATOM	2165	O1	AKG	313	4.799	15.240	54.659	1.000	20.82	
ANISOU	2165	O1	AKG	313	2957	2293	2659	514	-234	2 6 4
ATOM	2166	O2	AKG	313	6.643	14.144	53.787	1.000	17.79	

- 161 -

ANISOU	2166	O2	AKG	313	2407	1765	2587	74	-377	4	2	9
ATOM	2167	C2	AKG	313	6.867	15.178	55.844	1.000	20.08			
ANISOU	2167	C2	AKG	313	1997	2566	3068	-528	419	-3	9	9
ATOM	2168	O5	AKG	313	7.982	14.661	55.821	1.000	17.60			
ANISOU	2168	O5	AKG	313	2289	2066	2334	-314	226	-2	5	2
ATOM	2169	C3	AKG	313	6.272	16.080	56.872	1.000	21.69			
ANISOU	2169	C3	AKG	313	2751	1910	3581	240	62	-3	2	7
ATOM	2170	C4	AKG	313	7.318	16.741	57.716	1.000	21.50			
ANISOU	2170	C4	AKG	313	3246	1761	3160	199	-143	-1	8	5
ATOM	2171	C5	AKG	313	6.923	17.816	58.672	1.000	22.58			
ANISOU	2171	C5	AKG	313	3122	1840	3618	755	-495	-3	1	3
ATOM	2172	O3	AKG	313	7.754	18.591	59.124	1.000	27.48			
ANISOU	2172	O3	AKG	313	3581	2470	4389	-34	602	-1	2	6
ATOM	2173	O4	AKG	313	5.660	17.889	58.999	1.000	28.55			
ANISOU	2173	O4	AKG	313	3191	2809	4846	612	-246	-1	1	4
ATOM	2174	S	SO4	401	11.676	0.439	24.942	1.000	40.14			
ATOM	2175	O1	SO4	401	11.293	0.826	26.321	1.000	33.12			
ATOM	2176	O2	SO4	401	12.501	-0.829	25.014	1.000	35.79			
ATOM	2177	O3	SO4	401	10.430	0.189	24.129	1.000	54.89			
ATOM	2178	O4	SO4	401	12.500	1.520	24.329	1.000	44.80			
ATOM	2179	OW	HOH	501	-6.455	10.219	44.319	1.000	14.29			
ATOM	2180	OW	HOH	502	-10.520	18.612	50.560	1.000	12.86			
ATOM	2181	OW	HOH	503	-8.644	16.907	47.858	1.000	16.83			
ATOM	2182	OW	HOH	504	-10.313	20.800	43.074	1.000	16.10			
ATOM	2183	OW	HOH	505	-6.051	19.199	52.602	1.000	16.38			
ATOM	2184	OW	HOH	506	-6.873	24.642	47.100	1.000	20.55			
ATOM	2185	OW	HOH	507	10.676	-4.179	46.406	1.000	27.41			
ATOM	2186	OW	HOH	508	-0.077	21.786	40.872	1.000	15.22			
ATOM	2187	OW	HOH	509	5.761	13.656	46.041	1.000	17.40			
ATOM	2188	OW	HOH	510	29.135	31.449	51.982	1.000	18.40			
ATOM	2189	OW	HOH	511	26.032	32.724	52.741	1.000	17.03			
ATOM	2190	OW	HOH	512	10.965	32.371	46.000	1.000	16.70			
ATOM	2191	OW	HOH	513	23.871	24.457	58.649	1.000	18.71			
ATOM	2192	OW	HOH	514	26.353	29.063	50.326	1.000	18.96			
ATOM	2193	OW	HOH	515	23.191	33.106	53.153	1.000	20.41			
ATOM	2194	OW	HOH	516	21.429	11.721	55.329	1.000	18.39			
ATOM	2195	OW	HOH	517	9.122	15.567	53.585	1.000	24.87			
ATOM	2196	OW	HOH	518	27.843	17.352	53.437	1.000	27.76			
ATOM	2197	OW	HOH	519	-14.415	20.029	44.444	1.000	23.47			
ATOM	2198	OW	HOH	520	15.253	33.050	51.771	1.000	27.20			
ATOM	2199	OW	HOH	521	14.080	31.486	44.302	1.000	21.58			
ATOM	2200	OW	HOH	522	17.770	33.842	53.596	1.000	23.56			
ATOM	2201	OW	HOH	523	3.671	24.673	36.173	1.000	20.95			
ATOM	2202	OW	HOH	524	-15.683	28.618	52.535	1.000	24.05			
ATOM	2203	OW	HOH	525	-5.386	20.413	39.013	1.000	26.85			
ATOM	2204	OW	HOH	526	10.417	27.949	58.778	1.000	28.33			
ATOM	2205	OW	HOH	527	23.165	19.592	62.202	1.000	29.36			
ATOM	2206	OW	HOH	528	23.736	10.550	55.737	1.000	24.02			
ATOM	2207	OW	HOH	529	-1.662	28.650	42.485	1.000	21.62			
ATOM	2208	OW	HOH	530	-4.689	10.177	46.511	1.000	31.65			
ATOM	2209	OW	HOH	531	1.545	35.657	50.866	1.000	19.59			
ATOM	2210	OW	HOH	532	0.980	22.687	36.818	1.000	30.57			
ATOM	2211	OW	HOH	533	-12.450	16.848	56.071	1.000	28.42			
ATOM	2212	OW	HOH	534	-9.418	16.139	51.364	1.000	22.60			
ATOM	2213	OW	HOH	535	32.711	25.816	43.116	1.000	31.44			
ATOM	2214	OW	HOH	536	27.068	24.587	55.468	1.000	23.32			
ATOM	2215	OW	HOH	537	13.523	11.832	51.199	1.000	10.73			
ATOM	2216	OW	HOH	538	8.513	16.158	35.074	1.000	12.26			
ATOM	2217	OW	HOH	539	0.922	2.590	35.058	1.000	14.79			
ATOM	2218	OW	HOH	540	-1.548	3.709	34.484	1.000	14.25			
ATOM	2219	OW	HOH	541	11.711	16.898	30.416	1.000	17.84			

- 162 -

ATOM	2220	OW	HOH	542	15.389	11.536	32.065	1.000	17.88
ATOM	2221	OW	HOH	543	18.496	6.995	52.191	1.000	17.47
ATOM	2222	OW	HOH	544	19.848	22.580	35.334	1.000	17.28
ATOM	2223	OW	HOH	545	-0.387	4.787	41.967	1.000	13.22
ATOM	2224	OW	HOH	546	23.502	12.662	35.308	1.000	18.14
ATOM	2225	OW	HOH	547	10.332	25.236	33.926	1.000	19.05
ATOM	2226	OW	HOH	548	21.447	20.605	34.090	1.000	17.24
ATOM	2227	OW	HOH	549	8.164	7.685	27.077	1.000	25.40
ATOM	2228	OW	HOH	550	14.393	-5.127	40.321	1.000	15.88
ATOM	2229	OW	HOH	551	12.873	29.356	39.662	1.000	16.45
ATOM	2230	OW	HOH	552	11.974	24.144	58.426	1.000	19.71
ATOM	2231	OW	HOH	553	17.521	7.949	33.182	1.000	17.90
ATOM	2232	OW	HOH	554	3.401	2.691	43.340	1.000	23.76
ATOM	2233	OW	HOH	555	18.669	28.057	40.079	1.000	18.44
ATOM	2234	OW	HOH	556	10.827	12.928	30.017	1.000	19.57
ATOM	2235	OW	HOH	557	20.630	16.270	66.466	1.000	20.84
ATOM	2236	OW	HOH	558	11.315	20.266	64.044	1.000	21.62
ATOM	2237	OW	HOH	559	26.277	14.516	43.946	1.000	16.22
ATOM	2238	OW	HOH	560	9.616	15.488	32.365	1.000	19.40
ATOM	2239	OW	HOH	561	8.888	4.903	27.857	1.000	22.74
ATOM	2240	OW	HOH	562	20.496	-1.851	42.511	1.000	22.98
ATOM	2241	OW	HOH	563	17.033	29.415	38.332	1.000	26.36
ATOM	2242	OW	HOH	564	18.595	6.141	37.697	1.000	25.10
ATOM	2243	OW	HOH	565	22.446	13.893	31.420	1.000	29.00
ATOM	2244	OW	HOH	566	6.586	3.577	28.350	1.000	27.82
ATOM	2245	OW	HOH	567	6.250	20.077	30.961	1.000	23.27
ATOM	2246	OW	HOH	568	7.341	16.113	31.186	1.000	28.59
ATOM	2247	OW	HOH	569	16.090	32.070	42.552	1.000	33.08
ATOM	2248	OW	HOH	570	11.500	28.806	37.258	1.000	25.17
ATOM	2249	OW	HOH	571	12.901	26.768	58.591	1.000	28.58
ATOM	2250	OW	HOH	572	-17.071	17.043	50.450	1.000	28.82
ATOM	2251	OW	HOH	573	25.262	7.705	37.199	1.000	39.05
ATOM	2252	OW	HOH	574	32.884	26.440	51.734	1.000	29.03
ATOM	2253	OW	HOH	575	-1.199	19.088	42.527	1.000	14.86
ATOM	2254	OW	HOH	576	-4.389	33.026	63.392	1.000	29.56
ATOM	2255	OW	HOH	577	17.569	25.732	32.249	1.000	20.62
ATOM	2256	OW	HOH	578	-19.107	12.822	67.516	1.000	22.35
ATOM	2257	OW	HOH	579	29.333	19.198	51.975	1.000	22.51
ATOM	2258	OW	HOH	580	27.950	27.635	51.903	1.000	25.40
ATOM	2259	OW	HOH	581	-21.085	14.501	68.535	1.000	21.19
ATOM	2260	OW	HOH	582	1.529	17.378	33.953	1.000	25.29
ATOM	2261	OW	HOH	583	9.138	20.887	66.894	1.000	33.92
ATOM	2262	OW	HOH	584	-11.896	19.091	44.780	1.000	17.48
ATOM	2263	OW	HOH	585	6.382	12.597	43.347	1.000	22.09
ATOM	2264	OW	HOH	586	17.762	21.268	29.046	1.000	20.79
ATOM	2265	OW	HOH	587	-11.500	25.438	41.729	1.000	29.68
ATOM	2266	OW	HOH	588	7.877	1.046	29.689	1.000	27.70
ATOM	2267	OW	HOH	589	27.985	13.540	42.235	1.000	25.91
ATOM	2268	OW	HOH	590	1.276	14.852	34.021	1.000	20.41
ATOM	2269	OW	HOH	591	24.622	24.179	41.242	1.000	26.77
ATOM	2270	OW	HOH	592	0.404	14.096	36.006	1.000	27.92
ATOM	2271	OW	HOH	593	-2.835	36.981	57.827	1.000	31.86
ATOM	2272	OW	HOH	594	3.276	0.788	39.940	1.000	32.07
ATOM	2273	OW	HOH	595	11.025	-8.794	31.468	1.000	27.18
ATOM	2274	OW	HOH	596	6.301	2.276	42.639	1.000	29.74
ATOM	2275	OW	HOH	597	29.302	16.146	62.924	1.000	43.75
ATOM	2276	OW	HOH	598	19.039	20.964	67.011	1.000	30.85
ATOM	2277	OW	HOH	599	8.380	22.088	64.518	1.000	42.62
ATOM	2278	OW	HOH	600	21.480	10.826	34.742	1.000	25.74
ATOM	2279	OW	HOH	601	-2.907	21.956	38.566	1.000	30.92
ATOM	2280	OW	HOH	602	-3.928	29.841	43.352	1.000	43.96

- 163 -

ATOM	2281	OW	HOH	603	2.885	21.563	34.437	1.000	33.10
ATOM	2282	OW	HOH	604	11.801	6.043	25.270	1.000	38.18
ATOM	2283	OW	HOH	605	-1.019	17.197	40.472	1.000	18.48
ATOM	2284	OW	HOH	606	18.382	23.349	68.110	1.000	22.54
ATOM	2285	OW	HOH	607	-8.141	8.137	45.609	1.000	17.64
ATOM	2286	OW	HOH	608	5.022	2.667	51.700	1.000	24.29
ATOM	2287	OW	HOH	609	17.557	10.755	33.490	1.000	21.94
ATOM	2288	OW	HOH	610	11.222	1.201	49.675	1.000	20.61
ATOM	2289	OW	HOH	611	4.243	35.047	50.509	1.000	22.18
ATOM	2290	OW	HOH	612	11.103	4.031	56.082	1.000	22.08
ATOM	2291	OW	HOH	613	11.366	31.522	36.791	1.000	32.32
ATOM	2292	OW	HOH	614	-21.189	24.787	52.739	1.000	31.83
ATOM	2293	OW	HOH	615	7.847	-1.491	30.674	1.000	24.77
ATOM	2294	OW	HOH	616	19.041	11.937	31.445	1.000	25.97
ATOM	2295	OW	HOH	617	6.221	29.879	40.410	1.000	29.24
ATOM	2296	OW	HOH	618	17.266	5.933	35.280	1.000	23.72
ATOM	2297	OW	HOH	619	5.983	-7.215	28.510	1.000	28.19
ATOM	2298	OW	HOH	620	22.574	8.129	57.639	1.000	30.97
ATOM	2299	OW	HOH	621	2.553	7.806	60.287	1.000	28.77
ATOM	2300	OW	HOH	622	29.939	25.812	51.234	1.000	34.00
ATOM	2301	OW	HOH	623	2.205	34.823	53.632	1.000	25.88
ATOM	2302	OW	HOH	624	18.091	13.838	67.343	1.000	28.46
ATOM	2303	OW	HOH	625	8.342	3.195	58.475	1.000	26.84
ATOM	2304	OW	HOH	626	-16.086	18.427	42.790	1.000	31.11
ATOM	2305	OW	HOH	627	-2.098	13.445	35.620	1.000	27.48
ATOM	2306	OW	HOH	628	0.481	30.471	42.834	1.000	32.55
ATOM	2307	OW	HOH	629	13.368	33.845	42.899	1.000	28.70
ATOM	2308	OW	HOH	630	-13.792	14.642	51.533	1.000	25.58
ATOM	2309	OW	HOH	631	3.299	1.461	29.242	1.000	39.62
ATOM	2310	OW	HOH	632	-16.012	20.690	46.705	1.000	27.75
ATOM	2311	OW	HOH	633	19.606	8.142	31.259	1.000	27.02
ATOM	2312	OW	HOH	634	5.077	7.954	57.205	1.000	30.59
ATOM	2313	OW	HOH	635	-1.502	6.963	45.877	1.000	35.68
ATOM	2314	OW	HOH	636	9.974	17.449	38.804	1.000	21.84
ATOM	2315	OW	HOH	637	-22.829	12.836	67.228	1.000	25.04
ATOM	2316	OW	HOH	638	6.275	34.333	39.722	1.000	25.88
ATOM	2317	OW	HOH	639	2.248	19.798	56.051	1.000	26.67
ATOM	2318	OW	HOH	640	-20.552	17.013	67.454	1.000	31.34
ATOM	2319	OW	HOH	641	9.298	16.570	28.911	1.000	29.96
ATOM	2320	OW	HOH	642	-1.732	11.113	60.074	1.000	28.13
ATOM	2321	OW	HOH	643	34.157	23.604	44.657	1.000	36.36
ATOM	2322	OW	HOH	644	24.298	20.199	33.576	1.000	34.90
ATOM	2323	OW	HOH	645	13.803	-4.667	31.570	1.000	32.66
ATOM	2324	OW	HOH	646	6.295	-2.594	29.009	1.000	34.61
ATOM	2325	OW	HOH	647	5.623	37.039	49.318	1.000	28.08
ATOM	2326	OW	HOH	648	-18.805	19.286	46.868	1.000	38.32
ATOM	2327	OW	HOH	649	16.026	35.829	49.382	1.000	34.45
ATOM	2328	OW	HOH	650	-12.187	28.769	45.330	1.000	27.36
ATOM	2329	OW	HOH	651	21.344	5.778	55.101	1.000	27.43
ATOM	2330	OW	HOH	652	-1.848	2.125	32.240	1.000	32.02
ATOM	2331	OW	HOH	653	-14.568	18.811	55.775	1.000	29.95
ATOM	2332	OW	HOH	654	-8.655	26.254	38.301	1.000	32.07
ATOM	2333	OW	HOH	655	18.836	13.542	28.102	1.000	32.24
ATOM	2334	OW	HOH	656	16.217	14.669	25.619	1.000	33.35
ATOM	2335	OW	HOH	657	28.678	14.477	38.043	1.000	30.94
ATOM	2336	OW	HOH	658	-11.834	15.408	53.330	1.000	33.25
ATOM	2337	OW	HOH	659	-1.317	38.273	59.599	1.000	34.45
ATOM	2338	OW	HOH	660	8.784	13.918	28.681	1.000	33.62
ATOM	2339	OW	HOH	661	-3.058	14.508	47.405	1.000	28.79
ATOM	2340	OW	HOH	662	10.968	33.651	38.533	1.000	36.21
ATOM	2341	OW	HOH	663	28.960	21.602	53.665	1.000	29.25

- 164 -

ATOM	2342	OW	HOH	664	-10.709	26.808	39.175	1.000	42.71
ATOM	2343	OW	HOH	665	17.790	7.093	55.023	1.000	30.29
ATOM	2344	OW	HOH	666	6.404	24.865	29.848	1.000	34.55
ATOM	2345	OW	HOH	667	-15.418	19.777	58.341	1.000	33.82
ATOM	2346	OW	HOH	668	0.000	0.000	37.259	0.330	49.90
ATOM	2347	OW	HOH	669	19.652	24.610	33.660	1.000	31.77
ATOM	2348	OW	HOH	670	17.188	9.619	29.950	1.000	29.94
ATOM	2349	OW	HOH	671	17.708	2.958	28.338	1.000	34.94
ATOM	2350	OW	HOH	672	-0.059	3.652	30.079	1.000	32.23
ATOM	2351	OW	HOH	673	29.037	20.923	56.153	1.000	28.52
ATOM	2352	OW	HOH	674	-15.435	31.088	53.795	1.000	35.61
ATOM	2353	OW	HOH	675	-12.846	21.220	61.856	1.000	38.79
ATOM	2354	OW	HOH	676	10.299	39.666	49.554	1.000	40.30
ATOM	2355	OW	HOH	677	-5.921	28.822	41.521	1.000	34.01
ATOM	2356	OW	HOH	678	6.029	39.991	46.094	1.000	42.69
ATOM	2357	OW	HOH	679	35.052	23.156	52.356	1.000	40.17
ATOM	2358	OW	HOH	680	-12.008	38.355	51.601	1.000	35.18
ATOM	2359	OW	HOH	681	3.061	13.047	53.152	1.000	35.17
ATOM	2360	OW	HOH	682	1.379	2.075	27.532	1.000	46.38
ATOM	2361	OW	HOH	683	-0.516	-2.480	37.686	1.000	21.77
ATOM	2362	OW	HOH	684	4.567	10.310	43.503	1.000	24.86
ATOM	2363	OW	HOH	685	19.443	5.558	61.133	1.000	36.06
ATOM	2364	OW	HOH	686	3.205	29.499	40.656	1.000	36.99
ATOM	2365	OW	HOH	687	32.498	16.774	43.447	1.000	41.18
ATOM	2366	OW	HOH	688	28.166	23.113	57.593	1.000	35.56
ATOM	2367	OW	HOH	689	-17.023	23.220	46.759	1.000	30.05
ATOM	2368	OW	HOH	690	15.567	7.782	28.910	1.000	32.51
ATOM	2369	OW	HOH	691	11.780	30.287	57.203	1.000	33.34
ATOM	2370	OW	HOH	692	24.449	12.699	32.400	1.000	34.99
ATOM	2371	OW	HOH	693	26.200	25.005	57.918	1.000	39.38

CLAIMS

- 5 1. Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 10 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- 15 3. DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 20 4. Use of the three-dimensional structure of DAOCS for the modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
- 25 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the 7 α -methoxy group into cephamycin C.
- 30 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

7. Use as claimed in claim 5 for the modification of DAOCS, DACS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

5

8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

10

9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.

15

10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.

11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

20

12. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted:
25 Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above;

30

wherein the modifications:

AMENDED SHEET

- permit the enzyme to accept unnatural substrates; and/or
- enable the enzyme to produce unnatural products; and/or
- enhance the ability of the enzyme to produce useful products.

5 13. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, 10 Asn 304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above;

wherein the modifications:

- 15
- permit the enzyme to accept unnatural substrates; and/or
 - enable the enzyme to produce unnatural products; and/or enhance the ability of the enzyme to produce useful products.

14. An enzyme according to claim 12 or claim 13 which is a 20 mutant of DAOCS or DACS or DAOC/DACS.

15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues 25 specified in claims 12 and 13 is changed or deleted.

16. An enzyme as claimed in any one of claims 12-15, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic 30 interactions.

17. A gene encoding for the enzyme of any one of claims 12-16.
18. A micro-organism capable of expressing the gene of claim 17
5 under fermentation conditions.
19. Use of micro-organisms of claim 18 for the production of
beta-lactams of the penicillin or cephalosporin (including cepham) families.
20. Use as claimed in claim 19 wherein the micro-organism
10 contains another modified enzyme of the penicillin and cephalosporin
biosynthesis pathway including isopenicillin N synthase,
amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-
valine (ACV) synthetase.
- 15 21. A method which comprises using the three-dimensional
structure of DAOCS for determining or predicting the structure of another
related 2-oxoglutarate dependent enzyme or related enzyme not from the
penicillin and cephalosporin biosynthesis pathway, and using the structural
information so obtained for modifying the other enzyme or for designing an
20 inhibitor for the other enzyme; wherein the said other related enzyme is
modified, by deletion or addition or alteration; at one or more of the sites
defined in claim 12 or claim 13; or using the following information for the
design of an inhibitor: Asp185, His183 and His243 act as ligands to the
iron; Arg258 and Ser260 and the Fe bind the 2-oxoglutarate; Met180,
25 Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33,
Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are
important for the construction of the part of the active site binding 2-
oxoglutarate; and Arg160 and Arg162 are important for binding an amino
acid or peptide derived substrate.

22. A method as claimed in claim 21 wherein the said other related 2-oxoglutarate dependent enzyme or related enzyme is 1-aminocyclopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3 β -hydroxylase, hyoscyamine 6 β -hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ -butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavamate synthase, an oxygenase enzyme involved in the biosynthesis of carbapenems, the so called ethylene forming enzyme from *Pseudomonas syringae*, p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

23. A method as claimed in claim 21 or 22, wherein the said other related enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.

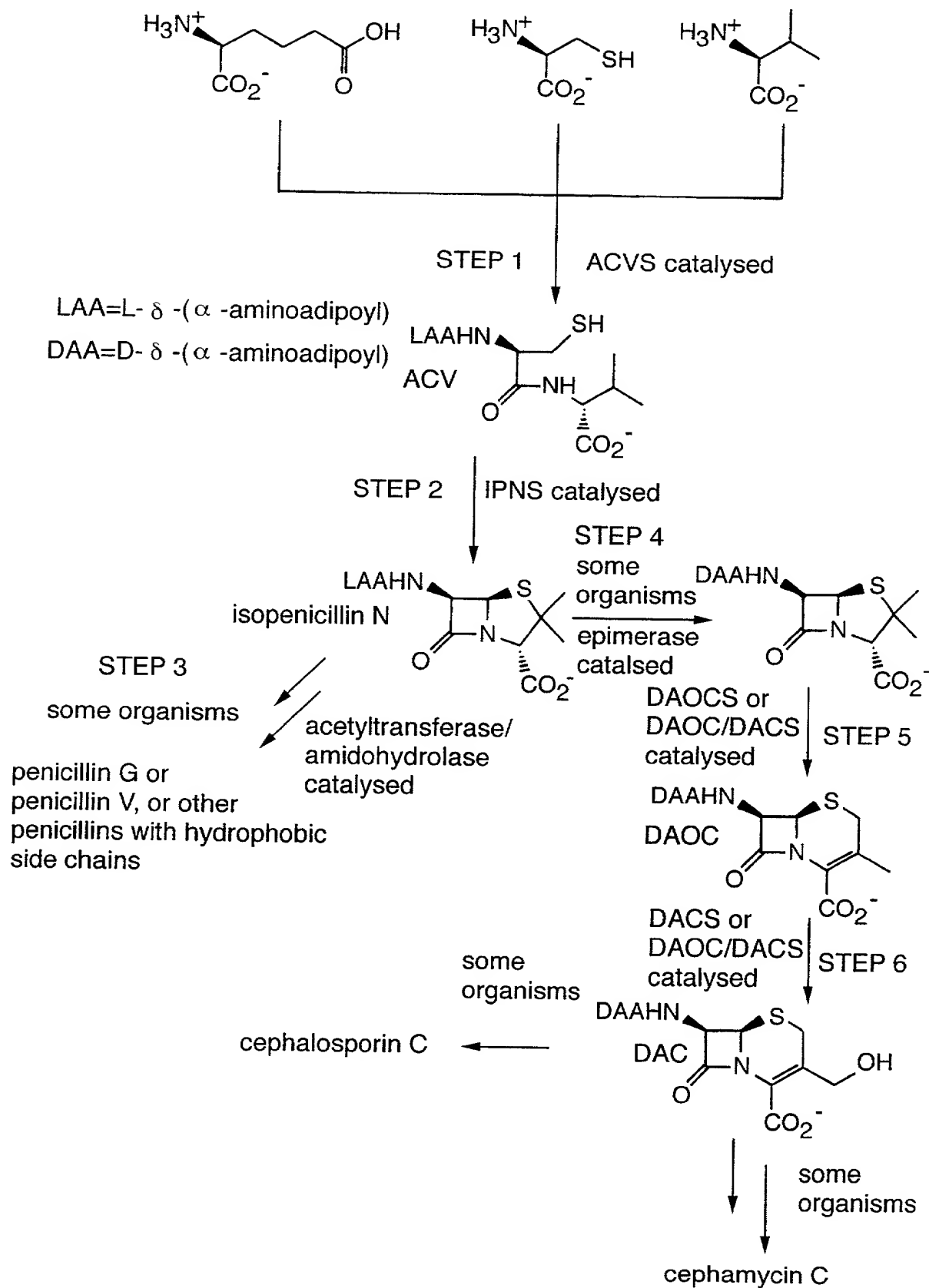
24. A method as claimed in claim 21 or 22, wherein the said other related enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.

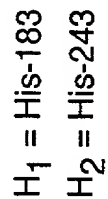
25. A method as claimed in claim 21 or 22, wherein the said other related enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

26. An enzyme as claimed in any one of claims 12 to 16, which has modifications at at least two of the said amino acid residues.

1/2

Fig.1.



[illegible]

INVENTOR DECLARATION

Attorney Docket No. P02005US0

As a below named inventor, I hereby declare that:

My residence, post office address and citizenship are as stated below next to my name.

I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled "MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE", the specification of which

(check one) ☐ is attached hereto.
☒ was filed on June 23, 2000 as PCT international application No. PCT/GB98/03860 and was amended on June 23, 2000.
 (if applicable)

I hereby state that I have reviewed and understand the contents of the above identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose information which is material to the examination of this application in accordance with Title 37, Code of Federal Regulations, § 1.56(a).

I hereby claim foreign priority benefits under Title 35, United States Code, § 119(a)-(d) or § 365(b) of any foreign application(s) for patent or inventor's certificate, or § 365(a) of any PCT international application which designated at least one country other than the United States of America, listed below and have also identified below any foreign application for patent or inventor's certificate, or of any PCT international application having a filing date before that of the application on which priority is claimed:

Prior Foreign Application(s)			Priority Claimed	
PCT/GB98/03860 (Number)	PCT (Country)	24 Dec. 1998 (Day/Month/Year Filed)	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No
9727370.0 (Number)	United Kingdom (Country)	24 Dec. 1997 (Day/Month/Year Filed)	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No
9813644.3 (Number)	United Kingdom (Country)	24 June 1998 (Day/Month/Year Filed)	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No

I hereby claim the benefit under Title 35, United States Code § 119(e) of any United States provisional application(s) listed below:

(Application Serial No.)	(Filing Date)

I hereby claim the benefit under Title 35, United States Code § 120 of any United States application(s), or § 365(b) of any PCT international application designating the United States of America, listed below and insofar as the subject matter of each of the claims of this application is not disclosed in the prior U.S. or PCT international application in the manner provided by the first paragraph of Title 35, U.S.C. § 112, I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations § 1.56(a) which occurred between the filing date of the prior application and the national or PCT international filing date of this application.

(Application Serial No.)	(Filing Date)	(Status) (patented, pending, abandoned)

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

Full Name of First Inventor <u>Christopher Joseph Schofield</u>	Inventor's Signature <i>C.J. Schofield</i>	Date 10/10/2000
Residence 19 Delamare Way, Cumnor Hill, Oxford, <u>Oxfordshire</u> OX2 9HZ, United Kingdom <i>GBX</i>		Citizenship UK
Post Office Address Same as above		

Full Name Second Inventor <u>Jack Edward Baldwin</u>	Inventor's Signature <i>J.E. Baldwin</i>	Date 11/10/2000
Residence Broom Hinksey Hill, Oxford, <u>Oxfordshire</u> OX1 5BH, United Kingdom <i>GBX</i>		Citizenship UK
Post Office Address Same as above		

Full Name Third Inventor <u>Peter L. Roach</u>	Inventor's Signature <i>P.L. Roach</i>	Date 18/8/00
Residence Exeter College, Oxford, <u>Oxfordshire</u> OX1 3DP, United Kingdom <i>GBX</i>		Citizenship UK
Post Office Address Same as above		

Full Name of Fourth Inventor <u>Matthew D. Lloyd</u>	Inventor's Signature <i>mat. Lloyd</i>	Date 23-8-00
Residence 8A North Wall <i>MOOR (MID)</i> Road, Oxford, <u>Oxfordshire</u> OX2 6UP, United Kingdom <i>GBX</i>		Citizenship UK
Post Office Address Same as above		

Full Name of Fifth Inventor <u>Karl Harlos</u>	Inventor's Signature <i>Karl Harlos</i>	Date 25-Sept-00
Residence 47 Purcell Road, Oxford, <u>Oxfordshire</u> OX3 0HD, United Kingdom <i>GBX</i>		Citizenship UK GERMAN
Post Office Address Same as above		

Full Name of Sixth Inventor <u>Inger Andersson</u>	Inventor's Signature <i>Inger Andersson</i>	Date 19/07/00
Residence Stabby Malmsvagen 8, 755 91 Uppsala, Sweden <i>SEX</i>		Citizenship Sweden
Post Office Address Same as above		

Full Name of Seventh Inventor <u>Janos Hajdu</u>	Inventor's Signature <i>Jan Hajdu</i>	Date 18/07/00
Residence Stabby Malmsvagen 8, 755 91 Uppsala, Sweden <i>SEX</i>		Citizenship Sweden HUNGARIAN
Post Office Address Same as above		

Full Name of Eighth Inventor Anke C. Terwisscha Van Scheltinga	Inventor's Signature <i>A. Terwisscha</i>	Date 18/7 2000
Residence Luthags Esplanaden 8A 752 25 Uppsala, Sweden	Citizenship Sweden DUTCH	
Post Office Address Same as above		

Full Name of Ninth Inventor Karin Valegard	Inventor's Signature <i>Karin Valegard</i>	Date 7/8 2000
Residence Prinsgatan 6, S-752 28 Uppsala, Sweden	Citizenship Sweden	
Post Office Address Same as above		

Full Name Tenth Inventor S. Ramaswamy	Inventor's Signature <i>S. Ram</i>	Date 10/AUG/2000
Residence Kopengatan 8, S-752 64 Uppsala, Sweden	Citizenship Sweden INDIAN	
Post Office Address Same as above		

POWER OF ATTORNEY

ISIS INNOVATION LIMITED, assignee of all right, title and interest in the enclosed patent application, hereby appoints the following agent(s) to prosecute this application and to transact all business in the Patent and Trademark Office connected therewith:

Ronald G. Bliss	Reg. No. 28,691
Paul E. Krieger	Reg. No. <u>25,886</u>
Robert J. Koch	Reg. No. <u>26,637</u>
Paul L. Deverter	Reg. No. <u>19,747</u>
James W. Repass	Reg. No. 30,487
Thomas D. Paul	Reg. No. 32,714
Marc L. Delflache	Reg. No. <u>28,942</u>
David L. Fox	Reg. No. 40,612
Jan K. Simpson	Reg. No. <u>33,283</u>
John M. Mings	Reg. No. 35,955
Mark E. Ungerman	Reg. No. <u>32,070</u>
Peter J. Davis	Reg. No. <u>36,119</u>
Scott Denko	Reg. No. <u>37,606</u>
Charles B. Walker, Jr.	Reg. No. <u>43,231</u>
Richard S. Zembek	Reg. No. <u>43,306</u>
Alberto Amatong	Reg. No. <u>41,580</u>
Gino Catena	Reg. No. <u>45,546</u>
Melissa Acosta	Reg. No. <u>45,872</u>
Melissa Schwaller	Reg. No. <u>46,089</u>
Melissa Sistrunk	Reg. No. <u>45,579</u>
Michael S. McCoy	Reg. No. <u>P-46,913</u>
Eric Hall	Reg. No. <u>P-46,751</u>

Address all correspondence to Patent Department; Fulbright & Jaworski L.L.P., 1301 McKinney, Suite 5100, Houston, Texas 77010-3095.

ISIS INNOVATION LIMITED



Dr. T. Cook
Managing Director
ISIS Innovation Ltd

DATE: 18-8-00